Quantum Condensed Matter Field Theory

Preface

The aim of this course is to provide a self-contained introduction to the basic tools and concepts of many-body quantum mechanics and quantum field theory, motivated by physical applications, and including the methods of second quantisation, the Feynman path integral and functional field integral. The course synopsis is outlined below. Items indicated by a † will either be covered in lectures (depending on time) or will be used as additional source material for problem sets and supervision. The italicised items represent particular mathematical concepts:

- ▷ Collective Excitations: From Particles to Fields: Linear harmonic chain and free scalar field theory; *functional analysis*; quantisation of the classical field; phonons; †relation to quantum electrodynamics; concepts of broken symmetry, collective modes, elementary excitations and universality. [3]

- ▷ Second Quantisation: Fock states; creation and annihilation operators for bosons and fermions; representations of one- and two-body operators; *canonical transformations*; Applications to phonons; the interacting electron gas; Wannier states, strong correlation and the Mott transition; quantum magnetism and spin wave theory; *spin representations*; †spin liquids; the weakly interacting Bose gas. [6]

- ▷ Path Integral Methods: Propagators and construction of the Feynman Path integral; *Gaussian functional integration and saddle-point analyses*; relation to semiclassics and statistical mechanics; harmonic oscillator and the single well; double well, instantons, and tunneling; †metastability and the fate of the false vacuum. [7]

- ▷ Many-Body Field Integral: Bose and Fermi coherent states; *Grassmann algebra*; coherent state Path integral; quantum partition function; Applications to Bogoluibov theory of the weakly interacting Bose gas and superfluidity; Cooper instability and the BCS condensate; Ginzburg-Landau phenomenology and the connection to classical statistical field theory, †Gauge theory and the Anderson-Higgs mechanism; †Resonance superfluidity in ultracold atomic gases and the BEC to BCS crossover, †Peierls instability. [8]

Course Objectives

From analytical dynamics and fluid mechanics, to electrodynamics and quantum mechanics, lectures can often leave an impression that to each problem in physics a specific and formal exact solution is at hand. Such misconceptions are often reinforced by the allure of sophisticated analytical machinery developed in courses devoted to mathematical methods. However, the limitations of a 'first-principles' or 'microscopic approach' is nowhere more exposed than in the study of strongly interacting classical and quantum *many-particle* systems. The aim of this course is to introduce modern methods of theoretical physics tailored to the description of collective phenomena where microscopic (and, often, perturbative) approaches fail. The fundamental concepts on which we rely are (broken) symmetries, collective modes, elementary excitations, and universality. The foundation of our approach will be functional methods of classical and quantum field theory.

To introduce the notion and significance of the quantum field, the first few introductory lectures involve the construction and quantisation of a classical continuum field theory starting from a discrete model of lattice vibrations. By the end of the course, we will see that this system provides a platform to describe the elementary excitations of spin-waves in a quantum antiferromagnet, excitations in a weakly interacting Bose gas, and the relativistic scalar field!

In the study of quantum many-body phenomena in both high energy and condensed matter physics, second quantisation provides a basic and common language. In the next few lectures, a formal introduction to this operator method is consolidated by applications to both fermionic and bosonic systems. Beginning with a study of the strongly interacting electron gas, we exploit the second quantisation to expose an instability towards the formation of an electron "solid phase" — out of which a magnetic state emerges. This application in turn motivates the investigation of the hydrodynamic or spin-wave spectrum of the quantum Heisenberg spin (anti)ferromagnet. We then close this section with a discussion of the weakly interacting dilute Bose gas.

As preparation for the field theory of the many-body system, the functional field integral method will be introduced and developed within the framework of the Feynman path integral. Emphasis will be given to the connection of the path integral to classical Lagrangian mechanics through the semi-classical expansion, as well as the relation to the quantum and classical statistical partition function through the Euclidean time action. The example of a single well and the instanton approach to the double well will be explored in lectures. Further applications to metastability and macroscopic quantum tunneling will be discussed depending on time.

In the study of both high energy and condensed matter physics, methods of quantum statistical field theory play a central role. Although modern field theory applications in the respective fields have developed to a high degree of specialisation, a common origin is shared. The aim of the remaining lectures is to introduce the subject of quantum and statistical field theory placing emphasis on generic concepts. Introducing the bosonic and fermionic coherent state, the first two lectures are concerned with the microscopic derivation of the coherent state path integral. The latter is applied to the weakly interacting Bose gas and the phenomenon of superfluidity. Continuing this theme, we then explore the pair instability of the interacting electron gas and the formation of the supercon-

ducting BCS condensate. Here, the connection between the effective BCS action and the Ginzburg-Landau theory of phase transitions and critical phenomena will be emphasised.

Problem Sets

The Problem sets represent an integral part of the course providing the means to reinforce key ideas as well as practice techniques. Problems indicated by a † symbol are regarded as particularly challenging.

Books

Several texts cover the introduction to second quantisation, path integrals and quantum field theory. However, one can draw great benefit by studying a variety of different texts. The bibliography below includes many books, some explicitly referenced in these lecture notes, others that I have found useful in preparing the course, and still others that are frequently mentioned but which I find less useful. A note has been included concerning their relevance and accessibility. Those books which would seem to be of particular use have been denoted by a "*". You will also, no doubt, find books *not* included in the this list which are both relevant and useful...

Alongside the literature, detailed lecture notes have been prepared to supplement the course. Although these lecture notes will include additional commentaries and examples not covered in the course, they are intended to complement the material contained in the lectures, and they *will not* form part of the examinable material for the course.

Bibliography

[1] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinskii, **Methods of Quantum Field Theory in Statistical Physics**, Dover Publications, Inc., 1975. *Advanced, historically significant, but somewhat out of date (only diagrammatics), and often overly concise.*

[2] A. Altland and B. D. Simons, **Condensed Matter Field Theory**, CUP Second Edition (2010). *Originally inspired by the preparation of this course, this text includes material that reaches far beyond these lectures.*

[3] N. W. Ashcroft and N. D. Mermin, **Solid State Physics**, Holt-Saunders International Eds. (1983). *Classical reference on solid state physics.*

[4] A. Auerbach, **Interacting Electrons and Quantum Magnetism**, Spinger-Verlag, New York (1994). *Tutorial discussion on applications of second quantisation and the path integral to problems in quantum magnetism.*

[5] *P. W. Anderson, **Concepts in Solids: Lectures of the Theory of Solids**, World-Scientific, Singapore (1997). *Exellent introduction to the concepts of elementary excitations in condensed matter physics.*

[6] P. W. Anderson, **Basic Notions in Condensed Matter Physics**, Benjamin (1984). *Inspirational but not tutorial — a highly subjective view of modern condensed matter physics from one of the most influential figures.*

[7] S. Coleman, **Aspects in Symmetry — Selected Erice Lectures** (CUP), 1985. *Chapter 5. has an excellent introduction to the subject of instantons — including applications to particle physics and cosmology — highly recommended.*

[8] A. Das, **Field Theory: A Path Integral Approach**, World Scientific Publishing, (1993). *A good, cheap, introduction to the path integral approach.*

[9] R. P. Feynman and A. R. Hibbs, **Quantum Mechanics and Path Integrals**, McGraw-Hill, New York, (1965). *A classic text: inevitably excludes a lot of modern material but still an excellent introduction to the Feynman path integral.*

[10] R. P. Feynman, **Statistical Mechanics**, Benjamin, New York, (1972). *Another classic text.*

[11] C. Kittel, **Quantum Theory of Solids**, Wiley (1963). *Not to be confused with the other famous text by the same author — good introduction to second quantisation and the physics of the weakly interacting electron gas.*

[12] *N. Nagaosa, **Quantum Field Theory in Condensed Matter Physics**, Sringer 1999. *An excellent and useful modern text. Short on detail but plenty of examples taken from condensed matter physics. See also the second volume in the series.*

[13] *J. W. Negele and H. Orland, **Quantum Many-Particle Systems**, Addison-Wesley Publishing, 1988. *Covers several core topics in this course including second quantisation and path integrals — high on detail, short on examples.*

[14] D. Pines and P. Nozières, **The Theory of Quantum Liquids — Neutral Fermi Liquids**, Addison-Wesley Publishing, NY (1989). *A classic text on solid state physics. Volume 2 is also interesting and relevant.*

[15] V. N. Popov, **Functional Integrals and Collective Excitations**, CUP, (1987). *Advanced and concise introduction to path integral methods generally in condensed matter physics — useful for much of the course.*

[16] *L. S. Schulman, **Techniques and Applications of Path Integration**, John Wiley & Sons, 1981. *Excellent introduction to the Feynman path integral.*

[17] A. M. Tsvelik, **Quantum Field Theory in Condensed Matter Physics**, (CUP) 1995. *A modern and entertaining discussion of applications of quantum field theory in condensed matter physics. Advanced, but useful as a source of inspiration.*

Contents

Chapter 1

From Particles to Fields

The aim of this section is to introduce the language and machinery of classical and quantum field theory through its application to the problem of lattice vibrations in a solid. In doing so, we will become acquainted with the notion of symmetry breaking, universality, elementary excitations and collective modes — concepts which will pervade much of the course.

1.1 Free scalar field theory: phonons

As a grossly simplified model of a (one-dimensional) quantum solid consider a chain of point particles of mass m (atoms) which are elastically connected by springs with spring constant k_s (chemical bonds) (see Fig. 1.1). The aim of this chapter will be to construct

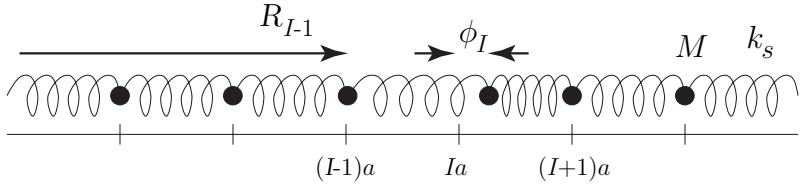


Figure 1.1: Toy model of a 1D solid – a chain of elastically bound massive point particles.

an effective quantum field theory of the vibrations of the one-dimensional solid. However, before doing so, we will first consider its classical behaviour. Analysing the classical case will not only tell us how to quantise the system, but also get us acquainted with some basic methodological concepts of field theory in general.

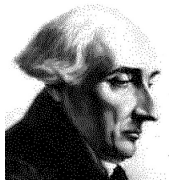
1.1.1 Classical chain

The classical **Lagrangian** of the N-atom chain is given by

$$L = T - V = \sum_{n=1}^{N} \left(\frac{m}{2} \dot{x}_n^2 - \frac{k_s}{2} (x_{n+1} - x_n - a)^2 \right), \tag{1.1}$$

where the first term accounts for the kinetic energy of the particles whilst the second describes their coupling.[1] For convenience, we adopt periodic boundary conditions such that $x_{N+1} = Na + x_1$. Anticipating that the effect of lattice vibrations on the solid is weak (i.e. long-range atomic order is maintained) we will assume that (a) the n-th atom has its equilibrium position at $\bar{x}_n \equiv na$ (with a the mean inter-atomic distance), and (b) that the deviation from the equilibrium position is small ($|x_n(t) - \bar{x}_n| \ll a$), i.e. the integrity of the solid is maintained. With $x_n(t) = \bar{x}_n + \phi_n(t)$ ($\phi_{N+1} = \phi_1$) the Lagrangian (1.1) takes the form,

Joseph-Louis Lagrange 1736-1813: A mathematician who excelled in all fields of analysis, number theory, and celestial mechanics. In 1788 he published *Mécanique Analytique*, which summarised all of the work done in the field of mechanics since the time of Newton, and is notable for its use of the theory of differential equations. In it he transformed mechanics into a branch of mathematical analysis.



$$L = \sum_{n=1}^{N} \left(\frac{m}{2} \dot{\phi}_n^2 - \frac{k_s}{2} \left(\phi_{n+1} - \phi_n \right)^2 \right).$$

Typically, one is not concerned with the behaviour of a given system on 'atomic' length scales. (In any case, for such purposes, a modelling like the one above would be much too primitive!) Rather, one is interested in **universal** features, i.e. experimentally observable behaviour that manifests itself on macroscopic length scales. For example, one might wish to study the specific heat of the solid in the limit of infinitely many atoms (or at least a macroscopically large number, $\mathcal{O}(10^{23})$). Under these conditions, microscopic models can usually be substantially simplified. In particular it is often permissible to subject a discrete lattice model to a **continuum limit**, i.e. to neglect the discreteness of the microscopic entities of the system and to describe it in terms of effective continuum degrees of freedom.

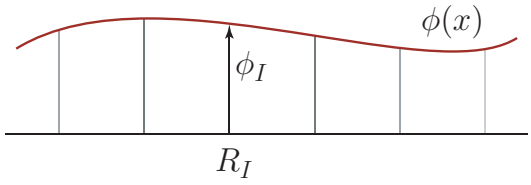


Figure 1.2: Continuum limit of harmonic chain.

In the present case, taking a continuum limit amounts to describing the lattice fluctuations ϕ_n in terms of *smooth functions* of a continuous variable x (Fig. 1.2). Clearly such a description makes sense only if relative fluctuations on atomic scales are weak (for otherwise the smoothness condition would be violated). Introducing continuum degrees of freedom $\phi(x)$, and applying a first order Taylor expansion,[2] we define

$$\phi_n \to a^{1/2} \phi(x)\Big|_{x=na}, \qquad \phi_{n+1} - \phi_n \to a^{3/2} \partial_x \phi(x)\Big|_{x=na}, \qquad \sum_{n=1}^{N} \longrightarrow \frac{1}{a} \int_0^L dx,$$

[1] In realistic solids, the inter-atomic potential is, of course, more complex than just quadratic. Yet, for "weak coupling", the harmonic (quadratic) contribution plays a dominant role. For the sake of simplicity we, therefore, neglect the effects caused by higher order contributions.

[2] Indeed, for reasons that will become clear, higher order contributions to the Taylor expansion do not contribute to the low-energy properties of the system where the continuum approximation is valid.

where $L = Na$ (not to be confused with the Lagrangian itself!). Note that, as defined, the functions $\phi(x,t)$ have dimensionality [Length]$^{1/2}$. Expressed in terms of the new degrees of freedom, the continuum limit of the Lagrangian then reads

$$L[\phi] = \int_0^L dx\ \mathcal{L}(\partial_x\phi, \dot{\phi}), \qquad \mathcal{L}(\partial_x\phi, \dot{\phi}) = \frac{m}{2}\dot{\phi}^2 - \frac{k_s a^2}{2}(\partial_x\phi)^2, \tag{1.2}$$

where the **Lagrangian density** $\mathcal{L}$ has dimensions [energy]/[length]. (Here, and hereafter, we will adopt the shorthand convention $\dot{O} \equiv \partial_t O$.) The **classical action** associated with the dynamics of a certain configuration ϕ is defined as

$$\boxed{S[\phi] = \int dt\ L[\phi] = \int dt \int_0^L dx\ \mathcal{L}(\partial_x\phi, \dot{\phi})} \tag{1.3}$$

We have thus succeeded in abandoning the N-point particle description in favour of one involving *continuous* degrees of freedom, a **(classical) field**. The dynamics of the latter is specified by the **functionals** L and S which represent the continuum generalisations of the discrete classical Lagrangian and action, respectively.

▷ Info. In the physics literature, mappings of functions into the real or complex numbers are generally called **functionals**. The argument of a functional is commonly indicated in angular brackets $[\,\cdot\,]$. For example, in this case, S maps the 'functions' $\partial_x\phi(x,t)$ and $\dot{\phi}(x,t)$ to the real number $S[\phi]$.

Although Eq. (1.2) specifies the model in full, we have not yet learned much about its actual behaviour. To extract concrete physical information from the action we need to derive **equations of motion**. At first sight, it may not be entirely clear what is meant by the term 'equations of motion' in the context of an infinite dimensional model. The answer to this question lies in Hamilton's extremal principle of classical mechanics:

Sir William Rowan Hamilton 1805-1865: A mathematician credited with the discovery of quaternions, the first non-commutative algebra to be studied. He also invented important new methods in Mechanics.

Suppose that the dynamics of a classical *point* particle with coordinate $x(t)$ is described by the classical Lagrangian $L(x,\dot{x})$, and action $S[x] = \int dt L(x,\dot{x})$. **Hamilton's extremal principle** states that the configurations $x(t)$ that are *actually realised* are those that extremise the action, viz. $\delta S[x] = 0$. This means that for any smooth curve, $y(t)$,

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon}(S[x+\epsilon y] - S[x]) = 0, \tag{1.4}$$

i.e. to first order in ϵ, the action has to remain invariant. Applying this condition, one finds that it is fulfilled if and only if $x(t)$ obeys **Lagrange's equation of motion** (a familiar result left here as a revision exercise)

$$\boxed{\frac{d}{dt}(\partial_{\dot{x}}L) - \partial_x L = 0} \tag{1.5}$$

In Eq. (1.3) we are dealing with a system of infinitely many degrees of freedom, $\phi(x,t)$. Yet Hamilton's principle is general, and we may see what happens if (1.3) is subjected to an extremal principle analogous to Eq. (1.4). To do so, we must implement the substitution $\phi(x,t) \to \phi(x,t) + \epsilon\eta(x,t)$ into Eq. (1.3) and demand that the contribution first order in ϵ vanishes. When applied to the specific Lagrangian (1.2), a substitution of the 'varied' field leads to

$$S[\phi + \epsilon\eta] = S[\phi] + \epsilon \int dt \int_0^L dx \left(m\,\dot{\phi}\,\dot{\eta} - k_s a^2\,\partial_x\phi\,\partial_x\eta \right) + \mathcal{O}(\epsilon^2).$$

Integrating by parts and demanding that the contribution linear in ϵ vanishes, one obtains

$$\int dt \int_0^L dx \left(m\ddot{\phi} - k_s a^2 \partial_x^2 \phi \right) \eta = 0.$$

(Notice that the boundary terms associated with both t abnd x vanish identically – think why.) Now, since $\eta(x,t)$ was defined to be an arbitrary smooth function, the integral above can only vanish if the term in parentheses is globally vanishing. Thus the equation of motion takes the form of a **wave equation**

$$\boxed{\left(m\partial_t^2 - k_s a^2 \partial_x^2\right)\phi = 0} \tag{1.6}$$

The solutions of Eq. (1.6) have the general form $\phi_+(x+vt) + \phi_-(x-vt)$ where $v = a\sqrt{k_s/m}$, and $\phi_\pm$ are arbitrary smooth functions of the argument. From this we can deduce that the low energy **elementary excitations** of our model are lattice vibrations propagating as **sound waves** to the left or right at a constant velocity v (see Fig. 1.3). Of course, the trivial behaviour of our model is a direct consequence of its simplistic definition — no dissipation, dispersion or other non-trivial ingredients. Adding these refinements leads to the general classical theory of lattice vibrations (see, e.g., Ref. [3]).

Figure 1.3: Schematic illustrating typical left and right moving excitations of the classical harmonic chain.

▷ INFO. **Functional Analysis**: Before proceeding further, let us briefly digress and revisit the derivation of the equations of motion (1.6). Although straightforward, the calculation was neither efficient, nor did it reveal general structures. In fact, what we did — expanding explicitly to first order in the variational parameter ϵ — had the same status as evaluating derivatives by explicitly taking limits: $f'(x) = \lim_{\epsilon\to 0}(f(x+\epsilon) - f(x))/\epsilon$. Moreover, the derivation made explicit use of the particular form of the Lagrangian, thereby being of limited use with regard to a general understanding of the construction scheme. Given the importance attached to extremal principles in all of field theory, it is worthwhile investing some effort in constructing a more efficient scheme for general variational analysis of continuum theories. In order to carry out

this programme we first need to introduce a mathematical tool of functional analysis, viz. the concept of functional differentiation.

In working with functionals, one is often concerned with how a given functional behaves under (small) variations of its argument function. In order to understand how answers to these types of questions can be systematically found, it is helpful to temporarily return to a discrete way of thinking, i.e. to interpret the argument f of a functional $F[f]$ as the limit $N \to \infty$ of a discrete vector $\mathbf{f} = \{f_n \equiv f(x_n), n = 1, \dots N\}$, where $\{x_n\}$ denotes a discretisation of the support of $\mathbf{f}$ (cf. Fig. 1.2 $\phi \leftrightarrow f$). Prior to taking the continuum limit, $N \to \infty$, $\mathbf{f}$ has the status of a N-dimensional vector and $F[\mathbf{f}]$ is a function defined over N-dimensional space. After the continuum limit, $\mathbf{f}$ becomes a function itself and $F[\mathbf{f}]$ becomes a functional.

Now, within the discrete picture it is clear how the variational behaviour of functions is to be analysed, e.g. the condition that, for all ϵ and all vectors $\mathbf{g}$, the linear expansion of $F[\mathbf{f} + \epsilon\mathbf{g}]$ ought to vanish, is simply to say that the total derivative, $\nabla F[\mathbf{f}]$, at $\mathbf{f}$ has to be zero. In practice, one often expresses conditions of this type in terms of a certain basis. For example, in a Cartesian basis of N unit vectors, $\hat{\mathbf{e}}_n,\ n = 1, \dots, N$,

$$F[\mathbf{f} + \epsilon\mathbf{g}] = F[\mathbf{f}] + \epsilon \sum_{n=1}^{N} (\partial_{f_n} F[\mathbf{f}]) g_n + \cdots, \qquad \partial_{f_n} F[\mathbf{f}] \equiv \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(F[\mathbf{f} + \epsilon \hat{\mathbf{e}}_n] - F[\mathbf{f}] \right). \tag{1.7}$$

The total derivative of F is zero, if and only if $\forall n$, $\partial_{f_n} F = 0$.

Taking the continuum limit of such identities will lead us to the concept of **functional differentiation**, a central tool in all areas of field theory. In the continuum limit, sums running from 1 to N become integrals. The nth unit vector $\hat{\mathbf{e}}_n$ becomes a function that is everywhere vanishing save at one point where it equals ∞, i.e. $\epsilon\hat{\mathbf{e}}_n \to \delta_x$, where the function $\delta_x(y) \equiv \delta(x-y)$.[3] Thus, the continuum limit of Eq. (1.7) reads

$$\begin{aligned} F[f + \epsilon g] &= F[f] + \epsilon \int dx \frac{\delta F[f]}{\delta f(x)} g(x) + \mathcal{O}(\epsilon^2) \\ \frac{\delta F[f]}{\delta f(x)} &\equiv \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(F[f + \epsilon \delta_x] - F[f] \right). \end{aligned} \tag{1.8}$$

Here the second line represents the definition of the functional derivative, i.e. the generalisation of a conventional partial derivative to infinitely many dimensions. Experience shows that it takes some time to get used to the concept of functional differentiation. However, after some practice it will become clear that this operation is not only extremely useful but also as easy to handle as conventional partial differentiation. In particular, all rules known from ordinary calculus (product-rule, chain-rule, etc.) immediately generalise to the functional case (as follows straightforwardly from the way the functional derivative has been introduced). For example, the generalisation of the standard chain rule,

$$\partial_{f_n} F[\mathbf{g}[\mathbf{f}]] = \sum_m \partial_{g_m} F[\mathbf{g}] \Big|_{\mathbf{g}=\mathbf{g}[\mathbf{f}]} \partial_{f_n} g_m[\mathbf{f}]$$

reads

$$\frac{\delta F[g[f]]}{\delta f(x)} = \int dy \left. \frac{\delta F[g]}{\delta g(y)} \right|_{g=g[f]} \frac{\delta g(y)[f]}{\delta f(x)}. \tag{1.9}$$

[3] If you find the singularity of the continuum version of the unit-vector difficult to accept, remember that the limit $\sum_n \langle \hat{\mathbf{e}}_n | \mathbf{f} \rangle = f_n \to \int dy\ \delta_x(y) f(y) = f(x)$ enforces $\delta_x(y) = \delta(x-y)$.

Furthermore, given some functional $F[f]$, we can Taylor expand it as

$$F[f] = F[0] + \int dx_1 \frac{\delta F[f]}{\delta f(x_1)} f(x_1) + \int dx_1 \int dx_2 \; \frac{1}{2} \frac{\delta^2 F[f]}{\delta f(x_2) \delta f(x_1)} f(x_1) f(x_2) + \cdots$$

Some basic definitions underlying functional differentiation as well as their finite dimensional counterparts are summarised in the following table:

entity	discrete	continuum
f	vector	function
$F[f]$	multi-dimensional function	functional
Cartesian basis	$\hat{\mathbf{e}}_n$	δ_x
'partial derivative'	$\partial_{f_n} F[\mathbf{f}]$	$\frac{\delta F[f]}{\delta f(x)}$

After this preparation, let us re-examine the extremal condition for a general action $S[x]$ by means of functional differentiation. As follows from the definition of the functional derivative (1.7), the action is extremal, if and only if $\forall x(t)$,

$$\frac{\delta S[x]}{\delta x(t)} = \int dt' \frac{\delta L(x(t'), \dot{x}(t'))}{\delta x(t)} = 0.$$

Employing the definition of the action in terms of the Lagrangian and applying the chain rule (1.9), we find

$$\int dt' \frac{\delta L(x(t'), \dot{x}(t'))}{\delta x(t)} = \int dt' \Big[\frac{\partial L(x(t'), \dot{x}(t'))}{\partial x(t')} \overbrace{\frac{\partial x(t')}{\partial x(t)}}^{\delta(t'-t)} + \frac{\partial L(x(t'), \dot{x}(t'))}{\partial \dot{x}(t')} \overbrace{\frac{\partial \dot{x}(t')}{\partial x(t)}}^{d_{t'}\delta(t'-t)} \Big],$$

From this result a rearrangement by integration obtains the familiar Euler-Lagrange equations

$$\frac{\delta S[x]}{\delta x(t)} = \frac{\partial L}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}(t)} \right) = 0.$$

It is left as a straightforward exercise to show that the general equations of motion of a classical continuum system with Lagrangian density $\mathcal{L}(\phi, \partial_x \phi, \dot{\phi})$ is given by

$$\boxed{\frac{\delta S[\phi]}{\delta \phi(x,t)} = \frac{\partial \mathcal{L}}{\partial \phi} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) - \frac{d}{dx} \left(\frac{\partial \mathcal{L}}{\partial (\partial_x \phi)} \right)} \tag{1.10}$$

Eq. (1.10) represents the generalisation of Lagrange's equation of motion of point mechanics to classical field theory (1.5). The particular application to the equations of motion of the simple phonon model (1.2) are illustrative of a *general principle*. All field theoretical models — be they classical or quantum — are represented in terms of certain actions whose extremal field configurations play a fundamental role.

After this digression, let us return to the discussion of the original model (1.2). As mentioned above, the classical vibrational physics of solids can be formulated in terms of models like (1.2) and its generalisations. On the other hand it is known (e.g. from the experimental study of specific heat [3]) that various aspects of the physics of lattices are non-classical and necessitate a quantum mechanical description. Hence, what is called for is an extension of the classical field theory to a quantum field theory.

1.1.2 Quantum Chain

The first question to ask is a conceptual one: how can a model like (1.2) be quantised in general? As a matter of fact there exists a standard procedure of quantising Lagrangian continuum theories which closely resembles the quantisation of point particle mechanics. The first step is to introduce canonical momenta conjugate to the continuum degrees of freedom (coordinates), ϕ, which will later be used to introduce canonical commutation relations. The natural generalisation of the definition $p_n \equiv \partial_{\dot{x}_n} L$ of point particle mechanics to a continuum suggests

$$\boxed{\pi(x) \equiv \frac{\partial \mathcal{L}}{\partial \dot{\phi}}} \tag{1.11}$$

or, more concisely, $\pi = \partial_{\dot{\phi}} \mathcal{L}$. In common with ϕ, the **canonical momentum**, π, is a continuum degree of freedom. At each space point it may take an independent value. From the Lagrangian, we can define the Hamiltonian,

$$\boxed{H[\phi, \pi] \equiv \int dx\ \mathcal{H}[\phi, \pi], \qquad \mathcal{H}[\phi, \pi] \equiv \pi \dot{\phi} - \mathcal{L}[\phi]}$$

where $\mathcal{H}$ represents the **Hamiltonian density**. (All the quantities appearing in $\mathcal{H}$ are to be expressed in terms of π and ϕ.) In particular, applied to the lattice model (1.2),

$$\mathcal{H}(\phi, \pi) = \frac{1}{2m}\pi^2 + \frac{k_s a^2}{2}(\partial_x \phi)^2.$$

where $\pi = m\dot{\phi}$.

In this form, the Hamiltonian can be quantised according to the rules: (i) promote the fields $\phi(x)$ and $\pi(x)$ to operators: $\phi \mapsto \hat{\phi}$, $\pi \mapsto \hat{\pi}$, and (ii) generalise the canonical commutation relations of single-particle quantum mechanics, $[\hat{p}_m, \hat{x}_n] = -i\hbar\delta_{mn}$, according to the relation[4]

$$\boxed{[\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar\delta(x - x')} \tag{1.12}$$

Operator-valued functions like $\hat{\phi}$ and $\hat{\pi}$ are generally referred to as **quantum fields**. Employing these definitions, we obtain the quantum Hamiltonian density

$$\hat{\mathcal{H}}[\hat{\phi}, \hat{\pi}] = \frac{1}{2m}\hat{\pi}^2 + \frac{k_s a^2}{2}(\partial_x \hat{\phi})^2. \tag{1.13}$$

The Hamiltonian above represents a quantum field theoretical *formulation* of the problem but not yet a *solution*. In fact, the development of a spectrum of methods for the analysis of quantum field theoretical models will represent a major part of this lecture course. At this point the objective is merely to exemplify how physical information can be extracted from models like (1.13).

[4]Note that the dimensionality of both the quantum and classical continuum fields is compatible with the dimensionality of the Dirac δ-function, $[\delta(x - x')] = [\text{Length}]^{-1}$.

As with any function, operator-valued functions can be represented in a variety of forms. In particular they can be subjected to Fourier expansion,

$$\left\{ \begin{matrix} \hat{\phi}_k \\ \hat{\pi}_k \end{matrix} \right. \equiv \frac{1}{L^{1/2}} \int_0^L dx \; e^{\{\mp ikx} \left\{ \begin{matrix} \hat{\phi}(x) \\ \hat{\pi}(x) \end{matrix} \right. , \qquad \left\{ \begin{matrix} \hat{\phi}(x) \\ \hat{\pi}(x) \end{matrix} \right. = \frac{1}{L^{1/2}} \sum_k e^{\{\pm ikx} \left\{ \begin{matrix} \hat{\phi}_k \\ \hat{\pi}_k \end{matrix} \right. , \tag{1.14}$$

where $\sum_k$ represents the sum over all Fourier coefficients indexed by quantised coordinates or "quasi-momenta" $k = 2\pi m/L$, $m \in \mathcal{Z}$. (Do not confuse the momenta k with the 'operator momentum' $\hat{\pi}$!) Note that the *real* classical field $\phi(x)$ quantises to a *Hermitian* quantum field $\hat{\phi}(x)$ implying that $\hat{\phi}_k = \hat{\phi}^\dagger_{-k}$ (and similarly for $\hat{\pi}_k$) — exercise. In the Fourier representation, the transformed field operators obey the canonical commutation relations (exercise)

$$\boxed{[\hat{\pi}_k, \hat{\phi}_{k'}] = -i\hbar\delta_{kk'}}$$

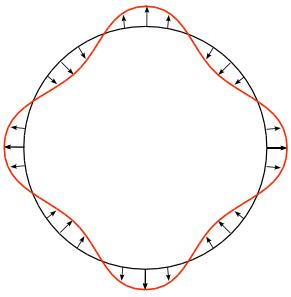
When expressed in the Fourier representation, making use of the identity

$$\int_0^L dx \, (\partial\hat{\phi})^2 = \sum_{k,k'} (ik\hat{\phi}_k)(ik'\hat{\phi}_{k'}) \overbrace{\frac{1}{L}\int_0^L dx \, e^{i(k+k')x}}^{\delta_{k+k',0}} = \sum_k k^2 \hat{\phi}_k \hat{\phi}_{-k} \left(\equiv \sum_k k^2 |\hat{\phi}_k|^2 \right)$$

together with a similar relation for $\int_0^L dx \, \hat{\pi}^2$, the Hamiltonian assumes the "near-diagonal" form[5]

$$\hat{H} = \sum_k \left[\frac{1}{2m} \hat{\pi}_k \hat{\pi}_{-k} + \frac{k_s a^2}{2} k^2 \hat{\phi}_k \hat{\phi}_{-k} \right] . \tag{1.15}$$

In this form, the Hamiltonian can be identified as nothing more than a superposition of independent **harmonic oscillators**.[6] This result is actually not difficult to understand (see figure): Classically, the system supports a discrete set of wave excitations, each indexed by a wave number $k = 2\pi m/L$. (In fact, we could have performed a Fourier transformation of the *classical* fields $\phi(x)$ and $\pi(x)$ to represent the Hamiltonian function as a superposition of classical harmonic oscillators.) Within the quantum picture, each of these excitations is described by an oscillator Hamiltonian with a k-dependent frequency. However, it is important not to confuse the atomic constituents, also oscillators (albethey coupled), with the independent *collective* oscillator modes described by $\hat{H}$.



[5] As a point of notation, when expressed in terms of a complete orthonormal basis $|m\rangle$, a general Hamiltonian can be expressed as a matrix, $H_{mn} = \langle m|\hat{H}|n\rangle$. In the eigenbasis $|\alpha\rangle$, the Hamiltonian is said to be diagonalised, viz. $H_{\alpha\beta} = \langle\alpha|\hat{H}|\beta\rangle = E_\alpha \delta_{\alpha\beta}$. In the present case, when expressed in the Fourier basis, the matrix elements correlate only k with $-k$.

[6] The only difference between (1.15) and the canonical form of an oscillator Hamiltonian $\hat{H} = \hat{p}^2/2m + m\omega^2\hat{x}^2/2$ is the presence of the sub-indices k and $-k$ (a consequence of $\hat{\phi}^\dagger_k = \hat{\phi}_{-k}$). As we will show shortly, this difference is inessential.

The description above, albeit perfectly valid, still suffers from a deficiency: Our analysis amounts to explicitly describing the low-energy excitations of the system (the waves) in terms of their microscopic constituents (the atoms). Indeed the different contributions to $\hat{H}$ keeps track of details of the microscopic oscillator dynamics of individual k-modes. However, it would be much more desirable to develop a picture where the relevant excitations of the system, the waves, appear as fundamental units, without explicit account of underlying microscopic details. (As with hydrodynamics, information is encoded in terms of collective density variables rather than through individual molecules.) As preparation for the construction of this improved formulation of the system, let us temporarily focus on a single oscillator mode.

▷ INFO. **Revision of the quantum harmonic oscillator:** Consider a standard harmonic oscillator (HO) Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \,.$$

The few first energy levels $\epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right)$ and the associated Hermite polynomial eigenfunctions are displayed schematically in Fig. 1.4. In quantum mechanics, the HO has, of course, the status of a single-particle problem. However, the fact that the energy levels are *equidistant* suggests an alternative interpretation: One can think of a given energy state ϵ_n as an accumulation of n elementary entities, or **quasi-particles**, each having energy $\hbar\omega$. What can be said about the features of these new objects? First, they are structureless, i.e. the only 'quantum number' identifying the quasi-particles is their energy $\hbar\omega$ (otherwise n-particle states formed of the quasi-particles would not be equidistant). This implies that the quasi-particles must be *bosons*. (The same state $\hbar\omega$ can be occupied by more than one particle — see Fig. 1.4.)

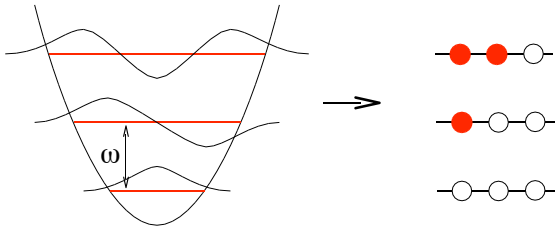


Figure 1.4: Low-lying energy levels/states of the harmonic oscillator Hamiltonian.

This idea can be formulated in quantitative terms by employing the formalism of ladder operators in which the operators $\hat{p}$ and $\hat{x}$ are traded for the pair of Hermitian adjoint operators $\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p})$, $\hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p})$. Up to a factor of i, the transformation $(\hat{x}, \hat{p}) \to (\hat{a}, \hat{a}^\dagger)$ is canonical, i.e. the new operators obey the canonical commutation relation

$$[\hat{a}, \hat{a}^\dagger] = 1 \,. \tag{1.16}$$

More importantly, the a-representation of the Hamiltonian is very simple, viz.

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) , \tag{1.17}$$

as can be checked by direct substitution. Suppose that we had been given a zero eigenvalue state $|0\rangle$ of the operator $\hat{a}$: $\hat{a}|0\rangle = 0$. As a direct consequence, $\hat{H}|0\rangle = (\hbar\omega/2)|0\rangle$, i.e. $|0\rangle$ is

identified as the ground state of the oscillator.[7] The complete hierarchy of higher energy states can now be generated by setting $|n\rangle \equiv (n!)^{-1/2}\,(\hat{a}^\dagger)^n|0\rangle$.

▷ EXERCISE. Using the canonical commutation relation, verify that $\hat{H}|n\rangle = \hbar\omega(n+1/2)|n\rangle$ and $\langle n|n\rangle = 1$.

So far, we have succeeded merely in finding yet another way of constructing eigenstates of the quantum HO problem. However, the real advantage of the a-representation is that it naturally affords a many-particle interpretation. Temporarily forgetting about the original definition of the oscillator, let us *declare* $|0\rangle$ to represent a 'vacuum' state, i.e. a state with no particles present. Next, imagine that $\hat{a}^\dagger|0\rangle$ is a state with a single featureless particle (the operator $\hat{a}^\dagger$ does not carry any quantum number labels) of energy $\hbar\omega$. Similarly, $(\hat{a}^\dagger)^n|0\rangle$ is considered as a many-body state with n particles, i.e. within the new picture, $\hat{a}^\dagger$ is an operator that creates particles. The total energy of these states is given by $\hbar\omega \times$ (occupation number). Indeed, it is straightforward to verify that $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$, i.e. the Hamiltonian basically counts the number of particles. While, at first sight, this may look unfamiliar, the new interpretation is internally consistent. Moreover, it fulfils our objective: it allows an interpretation of the excited states of the HO as a superposition of independent structureless entities.

The representation above illustrates the capacity to think about individual quantum problems in **complementary pictures**. This principle finds innumerable applications in modern condensed matter physics. To get used to it one has to realize that the existence of different interpretations of a given system is by no means heretic but, rather, is consistent with the spirit of quantum mechanics. Indeed, it is one of the prime principles of quantum theories that there is no such thing as 'the real system' which underpins the phenomenology. The only thing that matters is observable phenomena. For example, we will see later that the 'fictitious' quasi-particle states of oscillator systems *behave* as 'real' particles, i.e. they have dynamics, can interact, be detected experimentally, etc. From a quantum point of view there is actually no fundamental difference between these objects and the 'real' particles.

1.1.3 Quasi-Particle Interpretation of the Quantum Chain

WIth this background, we may return to the harmonic chain and transform the Hamiltonian (1.15) to a form analogous to (1.17) by defining the ladder operators[8]

$$\hat{a}_k \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_k + \frac{i}{m\omega_k}\hat{\pi}_{-k}\right), \qquad \hat{a}_k^\dagger \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_{-k} - \frac{i}{m\omega_k}\hat{\pi}_k\right),$$

where $\omega_k = v|k|$, and $v = a(k_s/m)^{1/2}$ denotes the classical sound wave velocity. With this definition, applying the commutation relations, one finds that the ladder operators obey

[7] ... as can be verified by explicit construction: Switching to a real space representation, the solution of the equation $[x + \hbar\partial_x/(m\omega)]\langle x|0\rangle = 0$ obtains the familiar ground state wavefunction $\langle x|0\rangle = \sqrt{2\pi\hbar/(m\omega)}e^{-m\omega x^2/2\hbar}$.

[8] As for the consistency of these definitions, recall that $\hat{\phi}_k^\dagger = \hat{\phi}_{-k}$ and $\hat{\pi}_k^\dagger = \hat{\pi}_{-k}$. Under these conditions the second of the definitions below indeed follows from the first upon taking the Hermitian adjoint.

the commutation relations (characteristic of Bose particles)

$$[a_k, a_{k'}^\dagger] = \frac{i}{2\hbar}\Big(\overbrace{[\hat\pi_{-k}, \hat\phi_{-k'}]}^{-i\hbar\delta_{kk'}} - [\hat\phi_k, \hat\pi_{k'}]\Big) = \delta_{kk'}, \tag{1.18}$$
$$[a_k, a_{k'}] = \frac{i}{2\hbar}\Big([\hat\pi_{-k}, \hat\phi_{k'}] + [\hat\phi_k, \hat\pi_{-k'}]\Big) = 0, \qquad [a_k^\dagger, a_{k'}^\dagger] = 0.$$

With this definition, one finds that the Hamiltonian assumes the diagonal form

$$\boxed{\hat H = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right)} \tag{1.19}$$

Equations (1.18) and (1.19) represent the final result of our analysis: The Hamiltonian $\hat H$ takes the form of a sum a set of harmonic oscillators with characteristic frequencies ω_k. In the limit $k \to 0$ (i.e. long wavelength), one finds $\omega_k \to 0$; excitations with this property are said to be **massless**.

An excited state of the system is indexed by a set $\{n_k\} = (n_1, n_2, \ldots)$ of quasi-particles with energy $\{\omega_k\}$. Physically, the quasi-particles of the harmonic chain are identified with the **phonon modes** of the solid. A comparison with measured phonon spectra (Fig. 1.5) reveals that, at low momenta, $\omega_k \sim |k|$ in agreement with our simplistic model (even in spite of the fact that the spectrum was recorded for a three-dimensional solid with non-trivial unit cell — universality!).

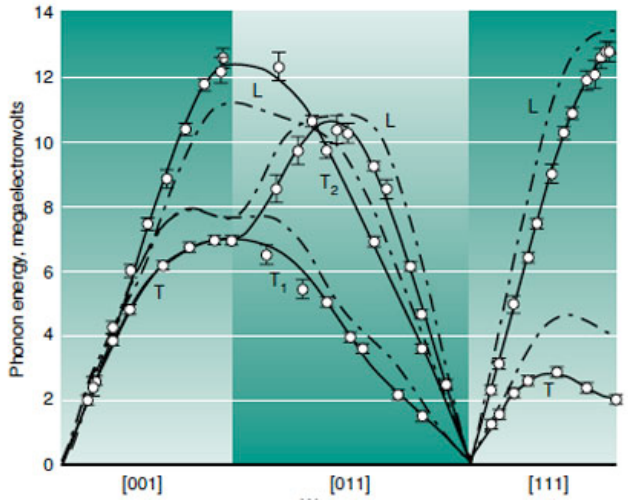


Figure 1.5: By applying energy and momentum conservation laws, one can determine the spectrum of the phonons from neutron scattering. The figure shows part of the phonon spectrum for plutonium. The measurement is sensitive to both longitudinal (L) and transverse (T) acoustic phonons. Notice that for small momenta, the dispersion is linear. (Figure from Joe Wong, Lawrence Livermore National Laboratory.)

1.2 †Quantum Electrodynamics (QED)

▷ Additional Example: As a second and important example of an analogous quantum field theory, consider electrodynamics. In this lecture course quantum electrodynamics (QED) will play comparatively little role. Nonetheless it is worthwhile to mention it briefly because

- ▷ QED is historically the oldest and still most successful field theory. (The QED result for the anomalous magnetic moment of the electron agrees with experiment up to a precision of $\mathcal{O}(10^{-6})$!)
- ▷ Quantised electromagnetic fields ($\rightarrow$ photons) play a significant role in many areas of condensed matter physics.

In the following short discussion we merely wish to illustrate the basic *principle* of field quantisation — in particular the parallels to the quantisation scheme employed in the previous example. For the *evaluation* of the resulting quantised theory we refer the reader to the literature. An excellent exposition of QED and its applications can be found, e.g., in Ryder's text on Quantum Field Theory.

The starting point of the quantisation scheme is again a classical variational principle. In other words we start out from a formulation where the *classical* physics of electromagnetic fields is derived from a Lagrangian function. As shown within the framework of classical relativistic electrodynamics the source-free Maxwell equations can be generated from the action

$$\boxed{S[A] = \int d^4x\, \mathcal{L}[A], \qquad \mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu},}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the electromagnetic field tensor, and $A = (\phi, \mathbf{A})^T$ is the 4-vector potential ($c = 1$). The Lagrangian above has the property of being (a) gauge invariant, and (b) exhibiting the solutions of the free Maxwell equations

$$\boxed{\partial_\mu F^{\mu\nu} = 0}$$

as its extremal field configurations.[9]

To work with the Lagrangian density $\mathcal{L}$ one needs to specify a gauge. (As a parenthetical remark we mention that the necessity to gauge fix is in fact a source of notorious difficulties in gauge field theories in general. However, these problems are of little concern for the present discussion.) Here we chose the so-called radiation or Coulomb gauge $\phi = 0$, $\nabla \cdot \mathbf{A} = 0$, thereby reducing the number of independent components of A from four to two. The next step towards a quantised theory is again to introduce canonical momenta. In analogy to section 1.1.2 we define $\pi^\mu = \partial_{\dot{A}_\mu} \mathcal{L}$ which leads to

$$\pi^0 = \partial_{\dot{A}_0} \mathcal{L} = 0, \qquad \pi^i = \partial_{\dot{A}_i} \mathcal{L} = \partial^0 A^i - \partial^i A^0 = E^i,$$

where $\mathbf{E}$ is the electric field.[10]

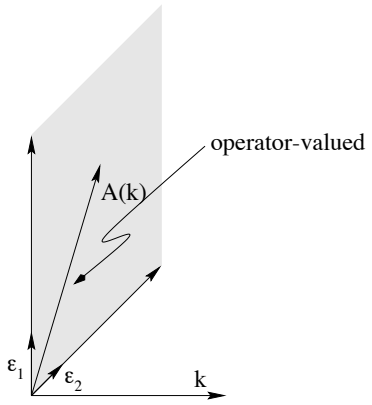
[9] To see this, one applies the usual variational principle, $\frac{\delta S[A]}{\delta A(x)} = 0$.

[10] The definitions above differ from the analogous equation (1.11) in so far as (a) the fields carry an additional discrete index $i = 1, \ldots 4$ — they are 'vector' rather than 'scalar' fields — and (b) that the indices appear as upper and sometimes as lower indices, where upper and lower indices are connected with each other by an application of the Minkowskii metric tensor. Both aspects are of little significance for the present discussion.

Quantising the field theory now again amounts to introducing operators $A_i \mapsto \hat{A}_i$, $\pi_i \mapsto \hat{\pi}_i$, as well as canonical commutation relations between $\hat{A}_i$ and $\hat{\pi}_j$. A natural *Ansatz* for the commutation relations would be

$$[\hat{A}_i(\mathbf{x},t),\hat{\pi}^j(\mathbf{x}',t)] = -[\hat{A}^i(\mathbf{x},t),\hat{\pi}^j(\mathbf{x}',t)] = i\delta_{ij}\delta(\mathbf{x}-\mathbf{x}'). \tag{1.20}$$

Yet a closer inspection reveals that these identities are in fact in conflict with the Coulomb gauge



$\nabla \cdot \mathbf{A} = 0$ (cf. Ryder, pp. 142). The way out is to replace δ_{ij} by a more general symmetric tensor. However as this complication does not alter the general *principle* of quantisation we do not discuss them any further here. The further construction of the theory is conceptually analogous to the phonon model and will be sketched only briefly.

Again one introduces momentum 'modes' by Fourier transforming the field:

$$\hat{A}_i(x) = \int \frac{d^3k}{(2\pi)^3 2k_0} \sum_{\lambda=1,2} \epsilon^{(\lambda)}(k) \left[a^{(\lambda)}(k)e^{-ikx} + \hat{a}^{(\lambda)\dagger}(k)e^{ikx} \right], \tag{1.21}$$

where $k^2 \equiv k_0^2 - \mathbf{k}^2 = 0$,[11] $\epsilon^{(\lambda)}(k)$ are polarisation vectors (cf. Fig. **??**) obeying $\mathbf{k} \cdot \epsilon^{(\lambda)}(k) = 0$ (Coulomb gauge!). The specific form of the integration measure follows from the general condition of relativistic invariance (cf. Ryder, pp. 143). Substituting this representation into the Hamilton operator of the field theory one obtains

$$\hat{H} = \sum_{\lambda} \int \frac{d^3k}{(2\pi)^3 2k_0} \frac{k_0}{2} a^{(\lambda)\dagger}(k) a^{(\lambda)}(k). \tag{1.22}$$

As Eq. (1.19), this is an oscillator type Hamiltonian. The difference is that the operators a generate oscillator quanta of the quantised electromagnetic field, so-called transverse **photons**, rather than phonons. Eq. (1.21) represents the decomposition of the free quantised vector potential in terms of photons. As with phonons, the oscillator quanta of the electromagnetic field can also be interpreted as particles. In this sense, the decomposition (1.21) represents the bridge between the wave and the particle description of electrodynamics. For discussions of the physical applications of the theory — in both high energy and condensed matter physics — we refer the reader to the literature, e.g. Ryder (high energy) and Ref. [1] (condensed matter).

[11] The condition $k \cdot k = 0$ follows from the Coulomb gauge formulation of Maxwell's equations, $\partial_\mu \partial^\mu A_\nu = 0$.

Chapter 2

Second Quantisation

In this section we introduce the method of second quantisation, the basic framework for the formulation of many-body quantum systems. The first part of the section focuses on methodology and notation, while the remainder is devoted to physically-motivated applications. Examples of the operator formalism are taken from various fields of quantum condensed matter.

2.1 Notations and Definitions

Second quantisation provides a basic and efficient language in which to formulate many-particle systems. As such, extensive introductions to the concept can be found throughout the literature (see, e.g., Feynman's text on Statistical Mechanics [10]). The first part of this section will be concerned with the introduction of the basic elements of second quantisation, while the remainder of this section will be concerned with developing fluency in the method by addressing a number of physical applications.

Let us begin by defining the (normalised) wavefunctions $|\psi_\lambda\rangle$ and corresponding eigenvalues ϵ_λ of the single-particle Hamiltonian $\hat{H}$, viz.

$$\hat{H}|\psi_\lambda\rangle = \epsilon_\lambda|\psi_\lambda\rangle.$$

With this definition, populating states 1 and 2, the symmetrised (normalised) two-particle wavefunction for fermions and bosons is respectively given by

$$\psi_{\substack{F\\B}}(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) \mp \psi_2(x_1)\psi_1(x_2)\right).$$

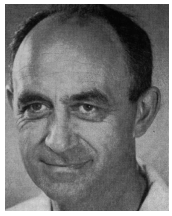
In the Dirac bracket representation, we can write

$$|1,2\rangle_{\substack{F\\B}} \equiv \frac{1}{\sqrt{2}}\left(|\psi_1\rangle \otimes |\psi_2\rangle \mp |\psi_2\rangle \otimes |\psi_1\rangle\right).$$

More generally, a *symmetrised* N-particle wavefunction of fermions ($\zeta = -1$) or bosons ($\zeta = +1$) is expressed in the form

$$\boxed{|\lambda_1, \lambda_2, \ldots \lambda_N\rangle \equiv \frac{1}{\sqrt{N!\prod_{\lambda=0}^{\infty} n_\lambda!}} \sum_{\mathcal{P}} \zeta^{\mathcal{P}} |\psi_{\lambda_{\mathcal{P}1}}\rangle \otimes |\psi_{\lambda_{\mathcal{P}2}}\rangle \ldots \otimes |\psi_{\lambda_{\mathcal{P}N}}\rangle}$$

where n_λ is the total number of particles in state λ (for fermions, Pauli exclusion enforces the constraint $n_\lambda = 0, 1$, i.e. $n_\lambda! = 1$) – see Fig. 2.1. The summation runs over all $N!$ permutations of the set of quantum numbers $\{\lambda_1, \ldots \lambda_N\}$, and $\mathcal{P}$ denotes the parity, defined as the number of transpositions of two elements which brings the permutation $(\mathcal{P}_1, \mathcal{P}_2, \cdots \mathcal{P}_N)$ back to the ordered sequence $(1, 2, \cdots N)$. Note that the summation over permutations is necessitated by quantum mechanical **indistinguishability**: for bosons/fermions the wavefunction has to be symmetric/anti-symmetric under particle exchange. It is straightforward to confirm that the prefactor $\frac{1}{\sqrt{N! \prod_\lambda n_\lambda!}}$ normalises the many-body wavefunction. In the fermionic case, the many-body wavefunction is known as a **Slater determinant**.



Enrico Fermi 1901-1954: 1938 Nobel Laureate in Physics for his demonstrations of the existence of new radioactive elements produced by neutron irradiation, and for his related discovery of nuclear reactions brought about by slow neutrons.

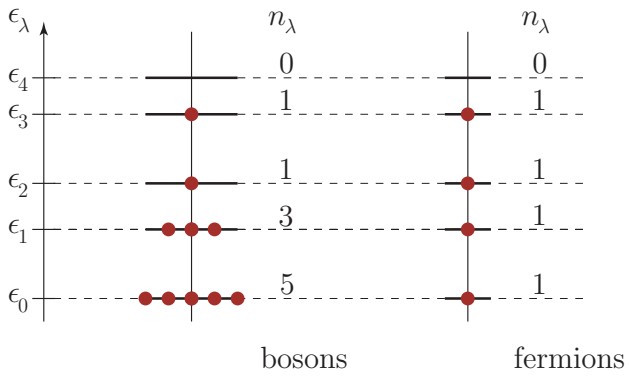


Figure 2.1: Schematic showing typical occupation numbers for a generic fermionic and bosonic system.

The expression above makes it clear that this 'first quantised' representation of the many-body wavefunction is clumsy. We will see that the second quantisation provides the means to heavily condense the representation. Let us define the **vacuum state** $|\Omega\rangle$, and introduce a set of **field operators** a_λ together with their adjoints $a_\lambda^\dagger$, as follows:[1]

$$\boxed{a_\lambda|\Omega\rangle = 0, \qquad \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} a^\dagger_{\lambda_N} \cdots a^\dagger_{\lambda_1}|\Omega\rangle = |\lambda_1, \lambda_2, \ldots \lambda_N\rangle} \tag{2.1}$$

Physically, the operator $a_\lambda^\dagger$ creates a particle in state λ while the operate a_λ annhilates it. These definitions are far from innocent and deserve some qualification. Firstly, in order not to be at conflict with the symmetry of the wavefunction, the operators a_λ have to fulfill the commutation relations,

$$\boxed{\left[a_\lambda, a^\dagger_\mu\right]_{-\zeta} = \delta_{\lambda,\mu}, \qquad \left[a_\lambda, a_\mu\right]_{-\zeta} = 0, \qquad \left[a^\dagger_\lambda, a^\dagger_\mu\right]_{-\zeta} = 0} \tag{2.2}$$

[1] As before, it will be convenient to represent these operators without a circumflex.

where $[\hat{A},\hat{B}]_{-\zeta} \equiv \hat{A}\hat{B} - \zeta\hat{B}\hat{A}$ is the commutator $\zeta = 1$ (anticommutator $\zeta = -1$) for bosons (fermions).[2] The most straightforward way to understand this condition is to check that the definition $|\lambda,\mu\rangle = a^\dagger_\lambda a^\dagger_\mu|\Omega\rangle$ and property $|\lambda,\mu\rangle = \zeta|\mu,\lambda\rangle$ in fact necessitate Eqs. (2.2). Yet even if (2.2) is understood, the definitions above remain non-trivial. Actually, quite a strong statement has been made: for *any* N, the N-body wavefunction can be generated by an application of a set of N-*independent* operators to a unique vacuum state. In order to check that Eqs. (2.1) and (2.2) actually represent a valid definition, including, for instance, the right symmetrisation and normalisation properties of N-body wave functions, various consistency checks have to be made.

Based on Eqs. (2.1) and (2.2), a formal definition of the general many-body or **Fock space** can now be given as follows. First define $\mathcal{F}_N$ to be the linear span of all N-particle states $|\lambda_1,\cdots\lambda_N\rangle = \frac{1}{\sqrt{\Pi_\lambda n_\lambda}} a^\dagger_{\lambda_N}\cdots a^\dagger_{\lambda_1}|\Omega\rangle$. The Fock space $\mathcal{F}$ is then defined as the direct sum $\oplus_{N=0}^\infty \mathcal{F}_N$ (see Fig. 2.2).[3] A general state $|\phi\rangle$ of the Fock space is, therefore,

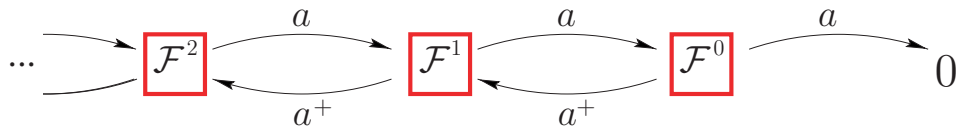


Figure 2.2: Visualisation of the generation of the Fock-subspaces $\mathcal{F}_N$ by repeated action of creation operators onto the vacuum space $\mathcal{F}_0$.

a linear combination of states with any number of particles. To turn these rather abstract definitions into a valuable tool for practical computation we need to put them into relation with standard operations performed in quantum mechanics. In particular we have to specify how changes from one single-particle basis $\{\lambda\}$ to another $\{\tilde{\lambda}\}$ effect the operator algebra $\{a_\lambda\}$, and in what way standard operators of (many-body) quantum mechanics can be represented in terms of the a_λ s:

▷ **Change of basis:** Using the resolution of identity, $\mathrm{id} = \sum_{\lambda=0}^\infty |\lambda\rangle\langle\lambda|$, the relations $|\tilde{\lambda}\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\tilde{\lambda}\rangle$, $|\lambda\rangle \equiv a^\dagger_\lambda|\Omega\rangle$, and $|\tilde{\lambda}\rangle \equiv a^\dagger_{\tilde{\lambda}}|\Omega\rangle$ immediately give rise to the transformation law

$$\boxed{a^\dagger_{\tilde{\lambda}} = \textstyle\sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a^\dagger_\lambda, \qquad a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda} \tag{2.3}$$

In many applications we are not dealing with a set of discrete quantum numbers (spin, quantised momenta, etc.), but rather with a continuum (a continuous position coordinate, say). In these cases, the quantum numbers are commonly denoted in a bracket notation $a_\lambda \rightsquigarrow a(x) = \sum_\lambda \langle x|\lambda\rangle a_\lambda$, and the summations appearing in the transformation formula above become integrals.

[2] As a convention, when unspecified by ζ, the notation $[\cdot,\cdot]$ will be used to denote the commutator and $\{\cdot,\cdot\}$ the anticommutator.

[3] Here, the symbol of the direct sum $\oplus$ is used to show that each "submodule" $\mathcal{F}_N$ is linearly independent.

Example: The transformation from the coordinate to the momentum representation in a finite one-dimensional system of length L would read

$$a_k = \int_0^L dx\ \langle k|x\rangle a(x), \qquad a(x) = \sum_k \langle x|k\rangle a_k,$$

where $\langle k|x\rangle \equiv \langle x|k\rangle^* = \frac{1}{L^{1/2}} e^{-ikx}$, cf. Fourier series expansion.

▷ **Representation of operators (one-body):** Single particle or one-body operators $\hat{\mathcal{O}}_1$ acting in a N-particle **Hilbert space**, $\mathcal{F}_N$, generally take the form $\hat{\mathcal{O}}_1 = \sum_{n=1}^N \hat{o}_n$, where $\hat{o}_n$ is an ordinary single-particle operator acting on the n-th particle. A typical example is the kinetic energy operator $\hat{T} = \sum_n \frac{\hat{p}_n^2}{2m}$, where $\hat{p}_n$ is the momentum operator acting on the n-th particle. Other examples include the one-particle potential operator $\hat{V} = \sum_n V(\hat{x}_n)$, where $V(x)$ is a scalar potential, the total spin-operator $\sum_n \hat{\mathbf{S}}_n$, etc. Since we have seen that, by applying field operators to the vacuum space, we can generate the Fock space in general and any N-particle Hilbert space in particular, it must be possible to represent any operator $\hat{\mathcal{O}}_1$ in an a-representation.

David Hilbert 1862-1943: His work in geometry had the greatest influence in that area after Euclid. A systematic study of the axioms of Euclidean geometry led Hilbert to propose 21 such axioms and he analysed their significance. He contributed to many areas of mathematics.

Now, although the representation of n-body operators is after all quite straightforward, the construction can, at first sight, seem daunting. A convenient way of finding such a representation is to express the operator in terms of a basis in which it is diagonal, and only later transform to an arbitrary basis. For this purpose it is useful to define the **occupation number operator**

$$\boxed{\hat{n}_\lambda = a_\lambda^\dagger a_\lambda} \tag{2.4}$$

with the property that, for bosons or fermions (exercise), $\hat{n}_\lambda\ (a_\lambda^\dagger)^n|\Omega\rangle = n\ (a_\lambda^\dagger)^n|\Omega\rangle$, i.e. the state $(a_\lambda^\dagger)^n|\Omega\rangle$ is an eigenstate of the number operator with eigenvalue n. When acting upon a state $|\lambda_1, \lambda_2, \cdots \lambda_N\rangle$, it is a straightforward exercise to confirm that the number operator simply counts the number of particles in state λ,

$$\hat{n}_\lambda|\lambda_1, \lambda_2, \cdots \lambda_N\rangle = a_\lambda^\dagger a_\lambda \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} a_{\lambda_N}^\dagger \cdots a_{\lambda_1}^\dagger|\Omega\rangle = \sum_{i=1}^N \delta_{\lambda\lambda_i}|\lambda_1, \lambda_2, \cdots \lambda_N\rangle.$$

Let us now consider a one-body operator, $\hat{\mathcal{O}}_1$, which is diagonal in the orthonormal basis $|\lambda\rangle$, $\hat{o} = \sum_\lambda o_\lambda|\lambda\rangle\langle\lambda|$, $o_\lambda = \langle\lambda|\hat{o}|\lambda\rangle$. With this definition, one finds

$$\begin{aligned}\langle\lambda_1', \cdots \lambda_N'|\hat{\mathcal{O}}_1|\lambda_1, \cdots \lambda_N\rangle &= \left(\sum_{i=1}^N o_{\lambda_i}\right)\langle\lambda_1', \cdots \lambda_N'|\lambda_1, \cdots \lambda_N\rangle \\ &= \langle\lambda_1', \cdots \lambda_N'|\sum_{\lambda=0}^\infty o_\lambda \hat{n}_\lambda|\lambda_1, \cdots \lambda_N\rangle.\end{aligned}$$

Since this equality holds for any set of states, we obtain the operator or second quantised representation $\hat{\mathcal{O}}_1 = \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} \langle\lambda|\hat{o}|\lambda\rangle a_\lambda^\dagger a_\lambda$. The result is straightforward; a one-body operator engages a single particle at a time — the others are just spectators. In the diagonal representation, one simply counts the number of particles in a state λ and multiplies by the corresponding eigenvalue of the one-body operator. Finally, by transforming from the diagonal representation to a general basis, one obtains the result,

Wolfgang Pauli 1900-1958: 1945 Nobel Laureate in Physics for the discovery of the Exclusion Principle, also called the Pauli Principle.

$$\boxed{\hat{\mathcal{O}}_1 = \sum_{\lambda\mu\nu} \langle\mu|\lambda\rangle o_\lambda \langle\lambda|\nu\rangle a_\mu^\dagger a_\nu = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle a_\mu^\dagger a_\nu} \tag{2.5}$$

Formally, the one-body operator, $\hat{\mathcal{O}}_1$, scatters a particle from a state ν into a state μ with probability amplitude $\langle\mu|\hat{o}|\nu\rangle$.

Examples: The **total spin operator** is given by

$$\hat{\mathbf{S}} = \sum_{\lambda\alpha\alpha'} a_{\lambda\alpha}^\dagger \mathbf{S}_{\alpha\alpha'} a_{\lambda\alpha'}, \qquad \mathbf{S}_{\alpha\alpha'} = \frac{1}{2}\boldsymbol{\sigma}_{\alpha\alpha'} \tag{2.6}$$

where $\alpha = \uparrow, \downarrow$ is the spin quantum number, λ denotes the set of additional quantum numbers (e.g. coordinate), and $\boldsymbol{\sigma}$ denotes the vector of Pauli spin matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.7}$$

i.e. $\hat{S}^z = \frac{1}{2}\sum_\lambda (\hat{n}_{\lambda\uparrow} - \hat{n}_{\lambda\downarrow})$, and $\hat{S}^+ = \sum_\lambda a_{\lambda\uparrow}^\dagger a_{\lambda\downarrow}$.

Second quantised in the position representation, the **one-body Hamiltonian** is given as a sum of kinetic and potential energy as (exercise)

$$\boxed{\hat{H} = \hat{T} + \hat{V} = \int dx\ a^\dagger(x) \left[\frac{\hat{p}^2}{2m} + V(x)\right] a(x)}$$

where $\hat{p} = -i\hbar\partial_x$. (Note that the latter is easily proved by expressing the kinetic energy in the diagonal (i.e. momentum) representation — see problem set.)

Finally, the **total occupation number operator** is defined as $\hat{N} = \int dx\ a^\dagger(x) a(x)$.

▷ **Representation of operators (two-body):** Two-body operators $\hat{\mathcal{O}}_2$ are needed to describe *pairwise interactions* between particles. Although pair-interaction potentials are straightforwardly included into *classical* many-body theories, their embedding into conventional many-body quantum mechanics is made awkward by particle indistinguishability. As compared to the conventional description, the formulation of interaction processes within the language of second quantisation is considerably more straightforward.

Initially, let us consider particles subject to the symmetric two-body potential $V(x, x') \equiv V(x', x)$. Acting on two-particle states, the operator is given by

$$\hat{V}^{(2)} = \frac{1}{2}\int dx \int dx'\ |x, x'\rangle V(x, x') \langle x, x'|. \tag{2.8}$$

Our aim is to find an operator $\hat{V}$ in second quantised form whose action on a many-body state gives

$$\hat{V}|x_1, x_2, \cdots x_N\rangle = \sum_{n<m}^{N} V(x_n, x_m)|x_1, x_2, \cdots x_N\rangle = \frac{1}{2}\sum_{n\neq m}^{N} V(x_n, x_m)|x_1, x_2, \cdots x_N\rangle.$$

Comparing this expressions with (2.8) one might immediately guess that

$$\hat{V} = \frac{1}{2}\int dx \int dx'\ a^\dagger(x)a^\dagger(x')V(x,x')a(x')a(x).$$

That this is the correct answer can be confirmed by applying the operator to a many-body state. We first note that

$$a(x')a(x)|x_1, x_2, \cdots x_N\rangle = a(x')\sum_{n=1}^{N}\zeta^{n-1}\delta(x-x_n)|x_1, x_2, \cdots (\text{no } x_n)\cdots x_N\rangle$$
$$= \sum_{n=1}^{N}\zeta^{n-1}\delta(x-x_n)\sum_{m=1,(m\neq n)}^{N}\eta_{mn}\delta(x'-x_m)|x_1, x_2, \cdots (\text{no } x_n, x_m)\cdots x_N\rangle$$

where

$$\eta_{mn} = \begin{cases} \zeta^{m-1} & \text{if } m < n \\ \zeta^{m} & \text{if } m > n \end{cases}.$$

Then, making use of the identity

$$a^\dagger(x)a^\dagger(x')a(x')a(x)|x_1, x_2, \cdots x_N\rangle$$
$$= \sum_{m\neq n}^{N}\zeta^{n-1}\eta_{mn}\delta(x-x_n)\delta(x'-x_m)|x, x', x_1, x_2, \cdots (\text{no } x_n, x_m)\cdots x_N\rangle$$
$$= \sum_{m\neq n}^{N}\zeta^{n-1}\eta_{mn}\delta(x-x_n)\delta(x'-x_m)|x_n, x_m, x_1, x_2, \cdots (\text{no } x_n, x_m)\cdots x_N\rangle$$
$$= \sum_{m\neq n}^{N}\delta(x-x_n)\delta(x'-x_m)|x_1, x_2, \cdots x_N\rangle,$$

multiplying by $V(x,x')/2$, and integrating over x and x', one confirms the validity of the expression. It is left as an exercise to confirm that the expression, $\frac{1}{2}\int dx \int dx'\, V(x,x')\hat{n}(x)\hat{n}(x')$ although a plausible candidate, does not reproduce the two-body operator.

More generally, turning to a non-diagonal basis, it is easy to confirm that a general two-body operator can be expressed in the form

$$\boxed{\hat{\mathcal{O}}_2 = \sum_{\lambda\lambda'\mu\mu'}\mathcal{O}_{\mu,\mu',\lambda,\lambda'}a^\dagger_{\mu'}a^\dagger_{\mu}a_{\lambda}a_{\lambda'}} \tag{2.9}$$

where $\mathcal{O}_{\mu,\mu',\lambda,\lambda'} \equiv \langle \mu, \mu' | \hat{\mathcal{O}}_2 | \lambda, \lambda' \rangle$.

In principle one may proceed in the same manner and represent general n-body interactions in terms of second quantised operators. However, as $n > 2$ interactions rarely appear, we refer to the literature for discussion.

This completes our formal introduction to the method of second quantisation. To make these concepts seem less abstract, the remainder of this section is concerned with the application of this method to a variety of problems.

2.2 Applications of Second Quantisation

Although the second quantisation is a representation and not a solution, its application often leads to a considerable simplification of the analysis of many-particle systems. To emphasize this fact, and to practice the manipulation of second quantised operators, we turn to several applications. The first example is taken from the physics of correlated electron systems, and will engage the manipulation of fermionic creation and annihilation operators. The second example involves the study of quantum magnetism within the framework of boson creation and annihilation operators. However, before getting to these applications, let us first go back and reinterpret our analysis of *phonon modes* in the quantum chain.

2.2.1 Phonons

Although, at the time, we did not specify in which Hilbert space the field operators a_k act, the answer is that the representation space is again a Fock space; this time a Fock space of phonons or, more formally, of oscillator states. In contrast to what we'll find for the fermion case below, the Fock space in the phonon problem does not have an *a priori* interpretation as a unification of physical N-particle spaces. However, outgoing from a vacuum state, it can be constructively generated by applying the oscillator creation operators $a_k^\dagger$ to a unique vacuum state:

▷ INFO. *Define* a ground or vacuum state $|\Omega\rangle$ by requiring that all operators a_k annihilate it. Next define $\mathcal{F}_0$ to be the space generated by $|\Omega\rangle$. We may then introduce a set of states $|k\rangle \equiv a_k^\dagger |\Omega\rangle,\ k = 0, 2\pi/L, \ldots$ by applying oscillator creation operators to the vacuum. Physically, the state $|k\rangle$ has the significance of a single harmonic oscillator quantum excited in mode k. In other words, all oscillator states $k' \neq k$ are in their ground state, whilst mode k is in the first exited state. The vector space generated by linear combinations of states $|k\rangle$ is called $\mathcal{F}_1$. This procedure can be iterated in an obvious manner. Simply define the space $\mathcal{F}_N$ to be generated by all states $a_{k_1}^\dagger \ldots a_{k_N}^\dagger |\Omega\rangle \equiv |k_1, \ldots, k_N\rangle$. The spaces $\mathcal{F}_N$ can be defined more concisely by saying that they are the eigenspaces of the occupation number operator with eigenvalue N. Finally, the Fock space is just the direct sum of all $\mathcal{F}_N$, $\mathcal{F} \equiv \oplus_{N=0}^{\infty} \mathcal{F}_N$. By construction, the application of any one $a_k^\dagger$ or a_k to states $\in \mathcal{F}$ does not leave $\mathcal{F}$. A closer analysis actually shows that the corresponding Fock space $\mathcal{F}$ represents a proper representation space for the operators a_k. A particle interpretation of the phonon states can now be naturally introduced by saying that the Fock space sector $\mathcal{F}_N$ represents a space of bosonic N-particle states. Application of $a_k^\dagger\,(a_k)$ to

a state $\in \mathcal{F}_N$ creates (annihilates) a particle (cf. Fig. 2.2).

2.2.2 Interacting Electron Gas

As a second example, we will cast the Hamiltonian of the interacting electron gas in second quantised form. To emphasize the utility of this approach, in the next section we will use it to explore the phase diagram of a strongly interacting electron gas. In doing so, we will uncover the limitations of the "nearly free electron theory" of metals.

As we have seen, in second quantised notation, the non-interacting Hamiltonian of a one-dimensional system of electrons subject to a lattice potential is given by

$$\hat{H}^{(0)} = \int dx \sum_{\sigma} c^{\dagger}_{\sigma}(x) \left[\frac{\hat{p}^2}{2m} + V(x) \right] c_{\sigma}(x),$$

where the fermionic electron field operators obey the anticommutation relations $[c_{\sigma}(x), c^{\dagger}_{\sigma'}(x')]_+ = \delta(x - x')\,\delta_{\sigma\sigma'}$. The field operators act on the 'big' many-particle Fock space, $\mathcal{F} = \oplus_{N=0}^{\infty} \mathcal{F}_N$. Each N-particle space $\mathcal{F}_N$ is spanned by states of the form $c^{\dagger}_{\sigma_N}(x_N) \cdots c^{\dagger}_{\sigma_1}(x_1)|\Omega\rangle$ where the 'no-particle' state or vacuum $|\Omega\rangle$ is annihilated by all operators $c_{\sigma}(x)$.

Applying a two-body Coulomb interaction potential, $\frac{1}{2}\sum_{i\neq j} \frac{e^2}{|x_i - x_j|}$, where x_i denotes the position of the i-th electron, the total many-body Hamiltonian takes the second quantised form

$$\boxed{\hat{H} = \hat{H}^{(0)} + \frac{1}{2} \int dx \int dx' \sum_{\sigma\sigma'} c^{\dagger}_{\sigma}(x) c^{\dagger}_{\sigma'}(x') \frac{e^2}{|x - x'|} c_{\sigma'}(x') c_{\sigma}(x)} \tag{2.10}$$

▷ Exercise. Setting $V(x) = 0$ and switching to the Fourier basis, reexpress the Coulomb interaction. Show that the latter is non-diagonal, and scatters electrons between different quasi-momentum states — see Fig. 2.3.

Having introduced both the field operators themselves and their representation spaces, we are in a position to point out certain conceptual analogies between the model theories discussed above. In each case we have described a physical system in terms of a theory involving a continuum of operators, $\hat{\phi}(x)$ (phonons) and $c_{\sigma}(x)$ (electrons). Of course there are also important differences between these examples. Obviously, in the phonon theory, we are dealing with bosons whilst the electron gas is fermionic. However, by far the most important difference is that the first example has been a **free field theory**. That means that the Hamiltonian contained field operators at quadratic order but no higher. As a rule, free field theories can be solved (in a sense that will become clear later on) straightforwardly. The

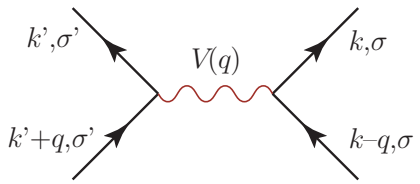


Figure 2.3: Feynman diagrammatic representation of the two-body Coulomb interaction.

fermionic model, however, represents a typical example of an interacting field theory. There are terms of fourth order in the field operators which arose from the Coulomb interaction term. As compared to free theories, the analysis of interacting theories is infinitely harder, a fact that will surely become evident later on.

To develop some fluency in the manipulation of second quantised field operators we will continue by exploring the '**atomic limit**' of a strongly interacting electron gas. In doing so, we will derive a model Hamiltonian which has served as a paradigm for the study of correlated electron systems.

2.2.3 Tight-binding theory and the Mott transition

According to the conventional band picture of non-interacting electrons, a system with a half-filled band of valence electron states is metallic. However, the strong Coulomb interaction of electrons can induce a phase transition to a (magnetic) insulating electron 'solid' phase (much as interactions can drive the condensation of a classical liquid into a solid). To explore the nature of this phenomenon, known as the **Mott transition** after Sir Neville Mott (formerly of the Cavendish Laboratory), it is convenient to reexpress the interacting Hamiltonian in a **tight-binding approximation**.

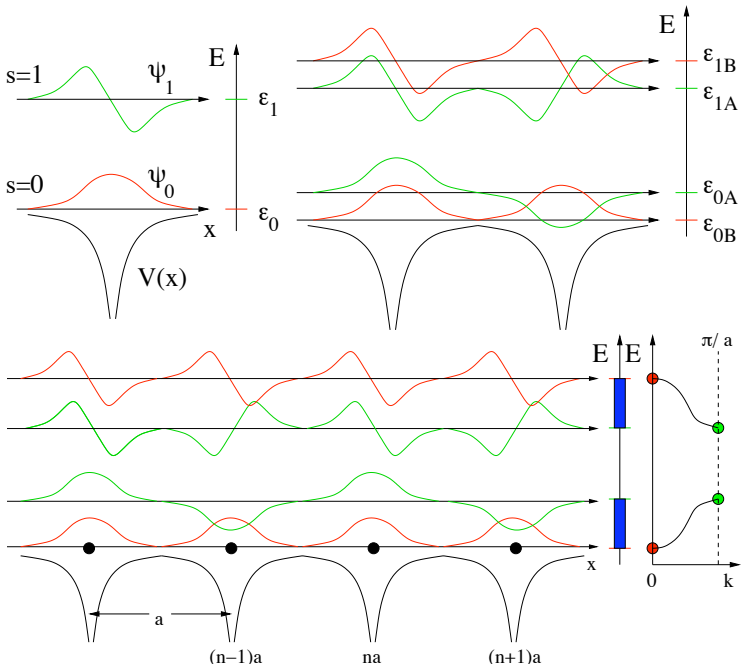
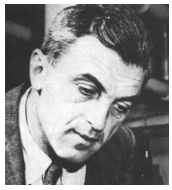


Figure 2.4: Infinitely separated, each lattice site is associated with a set of states, $s = 0, 1, \cdots$, bound to the ion core. Bringing together just two atoms, the orbitals weakly overlap and hybridise into bonding and anti-bonding combinations. Bringing together a well-separated lattice of atoms, each atomic orbital broadens into a delocalised band of Bloch states indexed by a quasi-momentum k from the Brillouin zone and an orbital or band index s.

To develop an effective Hamiltonian of the strongly interacting electron system we begin by considering a lattice of very widely spaced (almost isolated) atoms — the atomic

limit. In the simplest non-interacting picture, the overlap of the outermost electrons (albeit exponentially weak) leads to a hybridisation of the electronic orbitals and leads to the 'delocalisation' of a *narrow* band of extended states (see Fig. 2.4). These Bloch states $\psi_{ks}(x)$ of $\hat{H}^{(0)}$, which carry a quasi-momentum index k and a band or orbital index $s = 0, 1, \cdots$, provide a convenient basis with which to expand the interaction. We can, in turn, define a set of local **Wannier orbitals**



Felix Bloch 1905-1983: 1952 Nobel Laureate in Physics for the development (with Edward M. Purcell) of new methods for nuclear magnetic precision measurements and discoveries in connection therewith.

$$\overbrace{c^\dagger_{ns}|\Omega\rangle}^{|\psi_{ns}\rangle} \equiv \frac{1}{\sqrt{N}} \sum_{k\in[-\pi/a,\pi/a]}^{\text{B.Z.}} e^{ikna} \overbrace{c^\dagger_{ks}|\Omega\rangle}^{|\psi_{ks}\rangle}, \qquad |\psi_{ks}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-ikna}|\psi_{ns}\rangle$$

where N denotes the total number of primitive lattice sites (with periodic boundary conditions). Here the sum on k runs over the N k-points spanning the Brillouin zone, i.e. $k = 2\pi m/aN$ with integers $-N/2 < m \leq N/2$.

If the lattice is very widely spaced, the Wannier state ψ_{ns} will differ little from the s-th bound state of an isolated atom at $x = na$ (see Fig. 2.5). Restricting attention to the lowest band $s = 0$, and restoring the spin degrees of freedom σ, the field operators associated with the Wannier functions are defined by

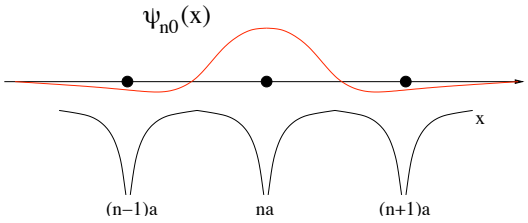


Figure 2.5: Diagram illustrating the weak overlap of Wannier states in the atomic limit.

$$\overbrace{c^\dagger_{n\sigma}|\Omega\rangle}^{|\psi_n\rangle} = \int_0^{L=Na} dx \overbrace{c^\dagger_\sigma(x)|\Omega\rangle}^{|x\rangle} \langle x|\psi_n\rangle,$$

i.e.

$$c^\dagger_{n\sigma} \equiv \int_0^L dx\ \psi_n(x) c^\dagger_\sigma(x), \qquad c^\dagger_\sigma(x) = \sum_{n=1}^{N} \psi^*_n(x) c^\dagger_{n\sigma}. \tag{2.11}$$

Physically, $c^\dagger_{n\sigma}$ can be interpreted as an operator creating an electron with spin σ at site n in the lowest band. Since the transformation (2.11) is unitary, it is straightforward to confirm that the operators $c_{n\sigma}$, and $c^\dagger_{n\sigma}$ obey fermionic anticommutation relations $[c_{n\sigma}, c^\dagger_{m\sigma'}]_+ = \delta_{\sigma\sigma'}\delta_{nm}$.

In the presence of a two-body Coulomb interaction, a substitution of the field operators in Eq. (2.10) by Wannier operators generates the generalised tight-binding Hamiltonian (exercise)

$$\boxed{\hat{H} = -\sum_{mn}\sum_{\sigma} t_{mn} c^\dagger_{m\sigma} c_{n\sigma} + \sum_{mnrs}\sum_{\sigma\sigma'} U_{mnrs}\ c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{r\sigma'} c_{s\sigma'}}$$

where the "hopping" matrix elements are given by

$$t_{mn} = -\langle\psi_m|\hat{H}^{(0)}|\psi_n\rangle = -\frac{1}{N}\sum_k e^{i(n-m)ka}\epsilon_k = t^*_{nm},$$

and the interaction parameters are set by (exercise)

$$U_{mnrs} = \frac{1}{2}\int_0^L dx \int_0^L dx'\ \psi^*_m(x)\psi^*_n(x')\frac{e^2}{|x-x'|}\psi_r(x')\psi_s(x).$$

Physically t_{mn} represents the probability amplitude for an electron to transfer (hop) from a site m to a site n.

▷ EXERCISE. Show that, in the Fourier basis, $c_{k\sigma} = \frac{1}{\sqrt{N}}\sum_n e^{-inka}c_{n\sigma}$, the non-interacting Hamiltonian takes the diagonal form $\hat{H}^{(0)} = \sum_k^{\text{B.Z.}} \epsilon_k c^\dagger_{k\sigma}c_{k\sigma}$.

Expressed in the Wannier basis, the representation above is exact (at least for states contained entirely within the lowest band). However, for a widely spaced lattice, most of the matrix elements of the general tight-binding model are small and can be neglected. Focusing on the most relevant:

▷ The **direct terms** $U_{mnnm} \equiv V_{mn}$ involve integrals over square moduli of Wannier functions and couple *density fluctuations* at different sites,

$$\sum_{m\neq n} V_{mn}\hat{n}_m\hat{n}_n,$$

where $\hat{n}_m = \sum_\sigma c^\dagger_{m\sigma}c_{m\sigma}$. Such terms have the capacity to induce *charge density* instabilities. Here we will focus on transitions to a magnetic phase where such contributions are inconsequential and can be safely neglected.

▷ A second important contribution derives from the **exchange coupling** which induces magnetic spin correlations. Setting $J^F_{mn} \equiv U_{mnmn}$, and making use of the identity $\sigma_{\alpha\beta}\cdot\sigma_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$, one obtains (exercise)

$$\sum_{m\neq n}\sum_{\sigma\sigma'} U_{mnmn}c^\dagger_{m\sigma}c^\dagger_{n\sigma'}c_{m\sigma'}c_{n\sigma} = -2\sum_{m\neq n} J^F_{mn}\left(\hat{\mathbf{S}}_m\cdot\hat{\mathbf{S}}_n + \frac{1}{4}\hat{n}_m\hat{n}_n\right).$$

Such contributions tend to induce weak **ferromagnetic coupling** of neighbouring spins (i.e. $J_F > 0$). Physically, the origin of the coupling is easily understood as deriving from a competition between kinetic and potential energies. By aligning with each other and forming a symmetric spin state, two electrons can reduce their potential energy arising from their mutual Coulomb repulsion. To enforce the anti-symmetry of the two-electron state, the orbital wavefunction would have to vanish at $x = x'$ where the Coulomb potential is largest. This mechanism is familiar from atomic physics where it is manifest as **Hund's rule**.

▷ However, in the **atomic limit** where the atoms are well-separated and the overlap between neighbouring orbitals is weak, the matrix elements t_{ij} and J^F_{ij} are exponentially small in the interatomic separation. By contrast the 'on-site' Coulomb or **Hubbard interaction**

$$\sum_m \sum_\sigma U_{mmmm} c^\dagger_{m\sigma} c^\dagger_{m\sigma'} c_{m\sigma'} c_{m\sigma} = U \sum_m \hat{n}_{m\uparrow} \hat{n}_{m\downarrow},$$

where $U \equiv 2U_{mmmm}$, increases as the atomic wavefunctions become more localised.

Therefore, dropping the constant energy off-set $\epsilon_0 = t_{nn}$, in the atomic limit, a strongly interacting many-body system of electrons can be described effectively by the (single-band) **Hubbard Hamiltonian**

$$\boxed{\hat{H} = -t \sum_{\langle mn \rangle} \sum_\sigma c^\dagger_{m\sigma} c_{n\sigma} + U \sum_m \hat{n}_{m\uparrow} \hat{n}_{m\downarrow}} \tag{2.12}$$

where we have introduced the notation $\langle mn \rangle$ to indicate a sum over neighbouring lattice sites, and $t = t_{mn}$ (assumed real and usually positive). In hindsight, a model of this structure could have been guessed on phenomenological grounds from the outset. Electrons tunnel between atomic orbitals localised on individual lattice sites and experience a local Coulomb interaction with other electrons.

Deceptive in its simplicity, the Hubbard model is acknowledged as a paradigm of strong electron correlation in condensed matter. Yet, after forty years of intense investigation, the properties of this seemingly simple model system — the character of the ground state and nature of the quasi-particle excitations — is still the subject of heated controversey (at least in dimensions higher than one — see below). Nevertheless, given the importance attached to this system, we will close this section with a brief discussion of the remarkable phenomenology that is believed to characterise the Hubbard system.

As well as dimensionality, the phase behaviour of the Hubbard Hamiltonian is characterised by three dimensionless parameters; the ratio of the Coulomb interaction scale to the bandwidth U/t, the particle density or filling fraction n (i.e. the average number of electrons per site), and the (dimensionless) temperature, T/t. The symmetry of the Hamiltonian under particle–hole interchange allows one to limit consideration to densities in the range $0 \leq n \leq 1$ while densities $1 < n \leq 2$ can be inferred by 'reflection'.

Focussing first on the low temperature system, in the dilute limit $n \ll 1$, the typical electron wavelength is greatly in excess of the particle separation and the dynamics is free. Here the local interaction presents only a weak perturbation and one can expect the properties of the Hubbard system to mirror those of the weakly interacting nearly free electron system. While the interaction remains weak one expects a metallic behaviour to persist. By contrast, let us consider the half–filled system where the average site occupancy is unity. Here, if the interaction is weak $U/t \ll 1$, one may again expect properties reminiscent of the weakly interacting electron system.[4] If, on the other hand, the interaction is very strong $U/t \gg 1$, site double occupancy is inhibited and electrons in the half–filled

[4] In fact, one has to exercise some caution since the commensurability of the Fermi wavelength with the lattice can initiate a transition to an insulating **spin density wave** state characterised by a small quasi-particle energy gap — the **Slater Instability**

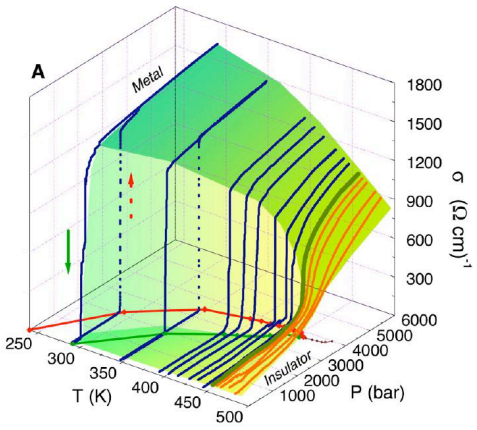


Figure 2.6: Conductivity of Cr–doped V_2O_3 as a function of decreasing pressure and temperature. At temperatures below the Mott–Hubbard transition point ($P_c = 3738\text{bar}, T_c = 457.5\text{K}$) the conductivity reveals hysteretic behaviour characteristic of a first order transition. Reproduced from Limelette *et al.*, *Universality and critical behavior at the Mott transition*, Science **302**, 89 (2003).

system become 'jammed': migration of an electron to a neighbouring lattice site necessitates site double occupancy incurring an energy cost U. In this strongly correlated phase, the mutual Coulomb interaction between the electrons drives the system from a metal to an insulator.

Sir Neville Mott 1905–1996: 1977 Nobel Laureate in Physics (with Philip W. Anderson and John H. van Vleck) for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems.

▷ INFO. Despite the ubiquity of the experimental phenomenon (first predicted in a celebrated work by Mott) the nature of the **Mott–Hubbard transtion** from the metallic to the insulating phase in the half–filled system has been the subject of considerable debate. In the original formulation, following a suggestion of Rudolf Peierls, Mott conceived of an insulator characterised by two 'Hubbard bands' with a bandwidth $\sim t$ separated by a charge gap U.[5] States of the upper band engage site double occupancy while those states that make up the lower band do not. The transition between the metallic and insulating phase was predicted to occur when the interaction was sufficiently strong that a charge gap develops between the bands. Later, starting from the weakly interacting Fermi–liquid, Brinkman and Rice[6] proposed that the transition was associated with the localisation of quasi–particles created by an interaction-driven renormalisation of the effective mass. Finally, a third school considers the transition to the Mott insulating phase as inexorably linked to the development of magnetic correlations in the weak coupling system — the Slater instability.

To summarise, we have shown how the method of second quantisation provides a useful and efficient way of formulating and investigating interacting electron systems. In the next section we will employ methods of second quantisation involving bosonic degrees of freedom to explore the collective excitations of quantum magnets.

[5] N. F. Mott, Proc. Roy. Soc. A **62**, 416 (1949) — for a review see, e.g. N. F. Mott, *Metal–Insulator transition*, Rev. Mod. Phys. **40**, 677 (1968) or N. F. Mott, *Metal–Insulator Transitions*, 2nd ed. (Taylor and Francis, London, 1990).

[6] W. Brinkman and T. M. Rice, *Application of Gutzwiller's variational method to the metal–insulator transition*, Phys. Rev. B **2**, 4302 (1970).

2.2.4 Quantum Spin Chains

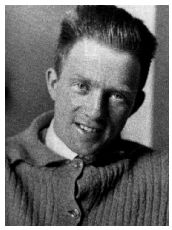
In the previous section, emphasis was placed on *charging effects* generated by Coulomb interaction. However, as we have seen, Coulomb interaction may also lead to the indirect generation of *magnetic* interactions of both ferromagnetic and antiferromagnetic character. To address the phenomena brought about by quantum magnetic correlations, it is instructive to begin by considering systems where the charge degrees of freedom are frozen and only spin excitations remain. Such systems are realized, for example, in Mott insulators where magnetic interactions between the local moments of localised electrons are mediated by virtual exchange processes between neighbouring electrons. Here, one can describe the magnetic correlations through models of localised quantum spins embedded on lattices. We begin our discussion with the ferromagnetic spin chain.

Quantum Ferromagnet

The quantum ferromagnetic chain is specified by the Heisenberg Hamiltonian

$$\boxed{\hat{H} = -J \sum_m \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}} \tag{2.13}$$

where $J > 0$, and $\hat{\mathbf{S}}_m$ represents the quantum mechanical spin operator at lattice site m. In section 2.1 (cf. Eq. (2.6)) the quantum mechanical spin was represented through an electron basis. However, one can conceive of situations where the spin sitting at site m is carried by a different object (e.g. an atom with non–vanishing magnetic moment). At any rate, for the purposes of our present discussion, we need not specify the microscopic origin of the spin. All we need to know is (i) that the lattice operators $\hat{S}^i_m$ obey the SU(2) commutator algebra (for clarity, we have set $\hbar = 1$ in this section)



Werner Heisenberg 1901–1976: 1932 Nobel Laureate in Physics "for the creation of quantum mechanics, the application of which has, *inter alia*, led to the discovery of the allotropic forms of hydrogen".

$$[\hat{S}^i_m, \hat{S}^j_n] = i\delta_{mn}\epsilon^{ijk}\hat{S}^k_n \tag{2.14}$$

characteristic of quantum mechanical spins, and (ii) that the total spin at each lattice site is S.[7]

Now, due to the positivity of the coupling constant J, the Hamiltonian favours configurations where the spins at neighbouring sites are aligned in the same direction (cf. Fig. 2.7). A ground state of the system is given by $|\Omega\rangle \equiv \otimes_m |S_m\rangle$, where $|S_m\rangle$ represents a state with maximal spin–z component: $\hat{S}^z_m|S_m\rangle = S|S_m\rangle$. We have written 'a' ground state instead of 'the' ground state because the system is highly degenerate: A simultaneous change of the orientation of all spins does not change the ground state energy, i.e. the system posesses a global spin rotation symmetry.

[7]Remember that the finite–dimensional representations of the spin operator are of dimension $2S + 1$ where S may be integer or half integer. While a single electron has spin $S = 1/2$, the total magnetic moment of electrons bound to an atom may be much larger.

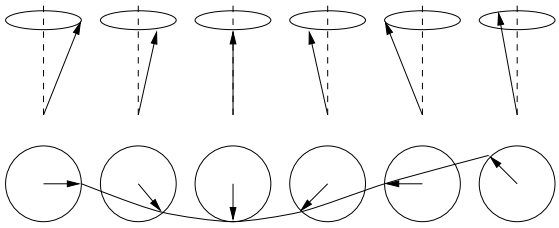


Figure 2.7: Schematic showing the spin configuration of an elementary spin-wave excitation from the spin polarized ground state.

▷ EXERCISE. Compute the energy expectation value of the state $|\Omega\rangle$. Defining *global* spin operator as $\hat{\mathbf{S}} \equiv \sum_m \hat{\mathbf{S}}_m$, consider the state $|\boldsymbol{\alpha}\rangle \equiv \exp(i(\pi/2)\boldsymbol{\alpha}\cdot\hat{\mathbf{S}})|\Omega\rangle$. Making use of the Baker-Hausdorff identity, $e^{i\lambda\hat{O}}\hat{A}e^{-i\lambda\hat{O}} = \hat{A} + i\lambda[\hat{O},\hat{A}] + \frac{(i\lambda)^2}{2!}[\hat{O},[\hat{O},\hat{A}]] + \cdots$ or otherwise, verify that the state $|\boldsymbol{\alpha}\rangle$ is degenerate with $|\Omega\rangle$. Explicitly compute the state $|(1,0,0)\rangle$. Convince yourself that for general $\boldsymbol{\alpha}$, $|\boldsymbol{\alpha}\rangle$ can be interpreted as a state with rotated quantisation axis.

As with our previous examples, we expect that a global continuous symmetry will involve the presence of energetically low–lying exciations. Indeed, it is obvious that in the limit of long wavelength λ, a weak distortion of a ground state configuration (cf. Fig. 2.7) will cost vanishingly small energy. To quantitatively explore the physics of these **spin–waves**, we adopt a 'semi–classical' picture, where the spin $S \gg 1$ is assumed to be large. In this limit, the rotation of the spins around the ground state configuration becomes similar to the rotation of a classical magnetic moment.

▷ INFO. To better understand the mechanism behind the **semi–classical approximation**, consider the Heisenberg uncertainty relation, $\Delta S^i \Delta S^j \leq |\langle[\hat{S}^i,\hat{S}^j]\rangle| = \epsilon^{ijk}|\langle\hat{S}^k\rangle|$, where ΔS^i is the root mean square of the quantum uncertainty of spin component i. Using the fact that $|\langle\hat{S}^k\rangle| \leq S$, we obtain for the relative uncertainty, $\Delta S^i/S$, $\frac{\Delta S^i}{S}\frac{\Delta S^j}{S} \leq \frac{S}{S^2} \overset{S\gg 1}{\longrightarrow} 0$, i.e. for $S \gg 1$, quantum fluctuations of the spin become less important.

In the limit of large spin S, and at low excitation energies, it is natural to describe the ordered phase in terms of small fluctuations of the spins around their expectation values (cf. the description of the ordered phase of a crystal in terms of small fluctuations of the atoms around the ordered lattice sites). These fluctuations are conveniently represented in terms of spin raising and lowering operators: with $\hat{S}^{\pm}_m \equiv S^x_m \pm iS^y_m$, it is straightforward to verify that

$$[\hat{S}^z_m,\hat{S}^{\pm}_n] = \pm\delta_{mn}\hat{S}^{\pm}_m, \qquad [\hat{S}^+_m,\hat{S}^-_n] = 2\delta_{mn}\hat{S}^z_m. \tag{2.15}$$

Application of $\hat{S}^{-(+)}_m$ lowers (raises) the z–component of the spin at site m by one. To actually make use of the fact that deviations around $|\Omega\rangle$ are small, a representation known as the **Holstein–Primakoff transformation**[8] was introduced in which the spin operators $\hat{S}^{\pm},\hat{S}$ are specified in terms of bosonic creation and annihilation operators $a^\dagger$ and a:

$$\hat{S}^-_m = a^\dagger_m(2S - a^\dagger_m a_m)^{1/2}, \qquad \hat{S}^+_m = (2S - a^\dagger_m a_m)^{1/2}a_m, \qquad \hat{S}^z_m = S - a^\dagger_m a_m$$

[8] T. Holstein and H. Primakoff, *Field dependence of the intrinsic domain magnetisation of a ferromagnet*, Phys. Rev. **58**, 1098 (1940).

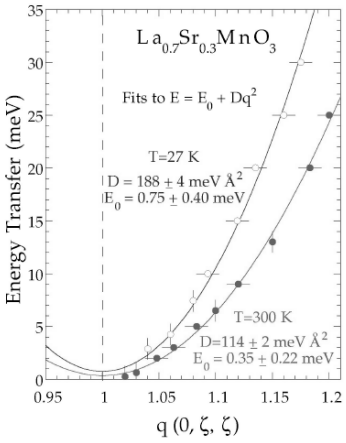


Figure 2.8: Measurements of the spin-wave dispersion relations for the ferromagnet $La_{0.7}Sr_{0.3}MnO_3$.

The utility of this representation is clear: When the spin is large $S \gg 1$, an expansion in powers of $1/S$ gives $\hat{S}^z_m = S - a^\dagger_m a_m$, $\hat{S}^-_m = (2S)^{1/2} a^\dagger_m + \mathcal{O}(S^{-1/2})$, and $\hat{S}^+_m = (2S)^{1/2} a_m + \mathcal{O}(S^{-1/2})$. In this approximation, the one-dimensional Hamiltonian takes the form

$$\begin{aligned}
\hat{H} &= -J \sum_m \left\{ \hat{S}^z_m \hat{S}^z_{m+1} + \frac{1}{2} \left(\hat{S}^+_m \hat{S}^-_{m+1} + \hat{S}^-_m \hat{S}^+_{m+1} \right) \right\} \\
&= -JNS^2 + JS \sum_m \left\{ a^\dagger_m a_m + a^\dagger_{m+1} a_{m+1} - \left(a^\dagger_m a_{m+1} + \text{h.c.} \right) \right\} + \mathcal{O}(S^0) \\
&= -JNS^2 + S \sum_m (a^\dagger_{m+1} - a^\dagger_m)(a_{m+1} - a_m) + \mathcal{O}(S^0).
\end{aligned}$$

Bilinear in Bose operators, the approximate Hamiltonian can be diagonalised by Fourier transformation. With periodic boundary conditions, $\hat{S}_{m+N} = \hat{S}_m$, $a_{m+N} = a_m$, defining

$$a_k = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{ikm} a_m, \qquad a_m = \frac{1}{\sqrt{N}} \sum_k^{\text{B.Z.}} e^{-ikm} a_k, \qquad [a_k, a^\dagger_{k'}] = \delta_{kk'},$$

the Hamiltonian for the one dimensional lattice system takes the form (exercise)

$$\boxed{\hat{H} = -JNS^2 + \sum_k^{\text{B.Z.}} \omega_k a^\dagger_k a_k + \mathcal{O}(S^0)} \tag{2.16}$$

where $\omega_k = 2JS(1 - \cos k) = 4JS \sin^2(k/2)$ represents the dispersion relation of the spin excitations. In particular, in the limit $k \to 0$, the energy of the elementary excitations vanishes, $\omega_k \to JSk^2$ (cf. Fig. 2.8). These massless low–energy excitations, known as **magnons**, describe the elementary spin–wave excitations of the ferromagnet. Taking into account terms at higher order in the parameter $1/S$, one finds interactions between the magnons.

Quantum Antiferromagnet

Having explored the low-energy excitation spectrum of the ferromagnet, we turn now to the spin S Heisenberg antiferromagnetic chain,

$$\hat{H} = J \sum_m \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}$$

where $J > 0$. Such local moment antiferromagnetic phases frequently occur in the arena of strongly correlated electron systems. Although the Hamiltonian differs from its ferromagnetic relative 'only' by a change of sign, the differences in the physics are drastic. Firstly, the phenomenology displayed by the antiferromagnetic Hamiltonian $\hat{H}$ depend sensitively on the geometry of the underlying lattice: For a **bipartite lattice**, i.e. one in which the neighbours of one sublattice A belong to the other sublattice B (cf. Fig. 2.9a), the ground states of the Heisenberg antiferromagnet are close[9] to a staggered spin configuration, known as a **Néel state**, where *all* neighbouring spins are antiparallel. Again the ground state is degenerate, i.e. a global rotation of all spins by the same amount does not change the energy. By contrast, on non–bipartite lattices such as the triangular lattice shown in Fig. 2.9b, no spin arrangement can be found wherein which each and every bond can recover the full exchange energy J. Spin models of this kind are said to be **frustrated**.

Louis Néel 1904–2000: 1970 Nobel Laureate in physics for fundamental work and discoveries concerning antiferromagnetism and ferrimagnetism which have led to important applications in solid state physics

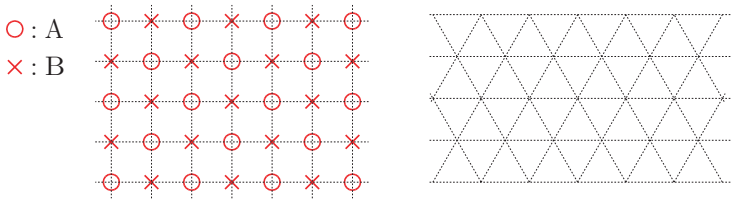


Figure 2.9: (a) Example of a two–dimensional bipartite lattice and (b) a non–bipartite lattice. Notice that, with the latter, no antiferromagnetic arrangement of the spins can be made that recovers the maximum exchange energy from each and every bond.

▷ Exercise. *Using only symmetry arguments*, specify one of the possible ground states of a classical three site triangular lattice antiferromagnet. (Note that the invariance of the Hamiltonian under a global rotation of the spins means that the there is manifold of continuous

[9]It is straightforward to verify that the classical ground state — the Néel state — is now not an exact eigenstate of the quantum Hamiltonian. The true ground state exhibits zero–point fluctuations reminiscent of the quantum harmonic oscillator or atomic chain. However, when $S \gg 1$, it serves as a useful reference state from which fluctuations can be examined.

degeneracy in the ground state.) Using this result, construct one of the classical ground states of the infinite triangular lattice.

Returning to the one–dimensional system, we first note that a chain is trivially bipartite. As before, our strategy will be to expand the Hamiltonian in terms of bosonic operators. However, before doing so, it is convenient to apply a canonical transformation to the Hamiltonian in which the spins on one sublattice, say B, are rotated through 180^o about the x–axis, i.e. $\hat{S}^x_B \mapsto S^x_B$, $S^y_B \mapsto -S^y_B$, and $S^z_B \mapsto -S^z_B$, i.e. when represented in terms of the new operators, the Néel ground state looks like a ferromagnetic state, with all spins aligned. We expect that a gradual distortion of this state will produce the antiferromagnetic analogue of the spin–waves discussed in the previous section.

Represented in terms of the transformed operators, the Hamiltonian takes the form

$$\hat{H} = -J \sum_m \left[\hat{S}^z_m \hat{S}^z_{m+1} - \frac{1}{2} \left(\hat{S}^+_m \hat{S}^+_{m+1} + \hat{S}^-_m \hat{S}^-_{m+1} \right) \right] .$$

Once again, applying an expansion of the Holstein–Primakoff representation, $S^-_m \simeq (2S)^{1/2} a^\dagger_m$, etc., one obtains the Hamiltonian

$$\hat{H} = -NJS^2 + JS \sum_m \left[a^\dagger_m a_m + a^\dagger_{m+1} a_{m+1} + a_m a_{m+1} + a^\dagger_m a^\dagger_{m+1} \right] + \mathcal{O}(S^0) .$$

At first sight the structure of this Hamiltonian, albeit bilinear in the Bose operators, looks akward. However, after Fourier transformation, $a_m = N^{-1/2} \sum_k e^{-ikm} a_k$, it assumes the more accessible form (exercise)

$$\hat{H} = -NJS(S+1) + JS \sum_k \begin{pmatrix} a^\dagger_k & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a^\dagger_{-k} \end{pmatrix} + \mathcal{O}(S^0),$$

where $\gamma_k = \cos k$.

Quadratic in the bosonic operators, the Hamiltonian can be again diagonalised by canonical transformation, i.e. a transformation of the field operators that preserves the commutation relations. In the present case, this is achieved by a **Bogoliubov transformation** .

N. N. Bogoliubov 1909-1992: Theoretical physcists aclaimed for his works in nonlinear mechanics, statistical physics, theory of superfluidity and superconductivity, quantum field theory, renormalization group theory, proof of dispersion relations, and elementary particle theory.

$$\begin{pmatrix} \alpha_k \\ \alpha^\dagger_{-k} \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} a_k \\ a^\dagger_{-k} \end{pmatrix} . \tag{2.17}$$

▷ Exercise. Construct the inverse transformation. Considering the commutation relations of the operators a_α, where $a_1 = a$ and $a_2 = a^\dagger$, explain why the Bogoliubov transformation is of the form of a Lorentz transformation. If operators a obeyed fermionic commutation relations, what form would the transformation take?

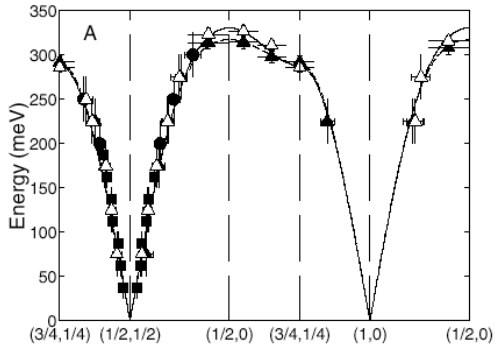


Figure 2.10: Experimentally obtained spin–wave dispersion of the high–T_c parent compound $LaCuO_4$ — a prominent spin 1/2 antiferromagnet. Figure reproduced from R. Coldea *et al.*, Phys. Rev. Lett. **86**, 5377 (2001).

Applying the Bogoliubov transformation, and setting $\tanh 2\theta_k = -\gamma_k$, the Hamiltonian assumes the diagonal form (exercise)

$$\boxed{\hat{H} = -NJS^2 + 2JS \sum_k |\sin k|\, \alpha_k^\dagger \alpha_k} \tag{2.18}$$

Thus, in contrast to the ferromagnet, the spin–wave excitations of the antiferromagnet exhibit a *linear dispersion* in the limit $k \to 0$. Surprisingly, although developed in the limit of large spin, experiment shows that even for $S = 1/2$ spin chains, the integrity of the linear dispersion is maintained (see Fig. 2.10).

2.2.5 Bogoliubov theory of the weakly interacting Bose gas

Ealier, we explored the influence of interactions on the electron gas. When interactions are weak, it was noted that the elementary collective excitations are reminiscent of the excitations of the free electron gas — the Fermi-liquid phase. When the interactions are strong, we discussed a scenario in which the electron liquid can condense into a solid insulating phase — the Mott transition. In the following section, we will discuss the properties of a quantum liquid comprised of Bose particles — the weakly interacting dilute Bose gas.

Let us consider a system of N Bose particles confined to a volume L^d and subject to the Hamiltonian

$$\boxed{\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2} \int d^d x\, d^d x'\; a^\dagger(\mathbf{x}) a^\dagger(\mathbf{x}') V(\mathbf{x}-\mathbf{x}') a(\mathbf{x}') a(\mathbf{x})}$$

where $\epsilon_{\mathbf{k}}^{(0)} = \frac{\hbar^2 \mathbf{k}^2}{2m}$, and $V(\mathbf{x})$ denotes a weak *repulsive* pairwise interaction. In the case of a Bose gas, this assumption is connected with the fact that, even for infinitesimal attractive forces, a Bose gas cannot stay dilute at low temperatures. In Fourier space, the corresponding two-body interaction can be expressed as (exercise)

$$\hat{H}_I = \frac{1}{2L^d} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{q}}\, a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} a_{\mathbf{k}'+\mathbf{q}},$$

where $a_{\mathbf{k}} = \frac{1}{L^{d/2}} \int d^d\mathbf{x}\, e^{i\mathbf{k}\cdot\mathbf{x}} a(\mathbf{x})$, and $V_{\mathbf{q}} = \int d^d\mathbf{x}\, e^{-i\mathbf{q}\cdot\mathbf{x}} V(\mathbf{x})$. In the following, we will be interested in the ground state and low-lying excitations of the dilute system. In this case, we may distill the relevant components of the interaction and considerably simplify the model.

In the ground state, the particles of an ideal (i.e. non-interacting) Bose gas *condense* into the lowest energy level. In a dilute gas, because of the weakness of the interactions, the ground state will differ only slightly from the ground state of the ideal gas, i.e. the number of particles N_0 in the condensate will still greatly exceed the number of particles in other levels, so that $N - N_0 \ll N$. Since the number of particles in the condensate is specified by the number operator $\hat{N}_0 = a^\dagger_{k=0} a_{k=0} = \mathcal{O}(N) \gg 1$, matrix elements of the Bose operators scale as $a_0 \sim O(\sqrt{N_0})$.[10] This means that, from the whole sum in the interaction, it is sufficient to retain only those terms which involve interaction with the condensate itself. Taking $V_{\mathbf{q}} = V$ constant, one obtains (exercise)

$$\hat{H}_I = \frac{V}{2L^d}\hat{N}_0^2 + \frac{V}{L^d}\hat{N}_0 \sum_{\mathbf{k}\neq 0} \left[a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}} a_{-\mathbf{k}} + \frac{1}{2}\left(a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} \right) \right] + \mathcal{O}(N_0^0).$$

Terms involving the excited states of the ideal gas have the following physical interpretation:

- ▷ $V a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$ represents the 'Hartree-Fock energy' of excited particles interacting with the condensate;[11]
- ▷ $V(a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}})$ represents creation or annihilation of excited particles from the condensate. Note that, in the present approximation, the total number of particles is not conserved.

Now, using the identity $N = \hat{N}_0 + \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$ to trade for $\hat{N}_0$, the total Hamiltonian takes the form

$$\hat{H} = \frac{VnN}{2} + \sum_{\mathbf{k}\neq 0} \left[\left(\epsilon^{(0)}_{\mathbf{k}} + Vn \right) \left(a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}} a_{-\mathbf{k}} \right) + \frac{Vn}{2} \left(a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} \right) \right],$$

where $n = N/L^d$ represents the total number density. This result may be compared with that obtained for the Hamiltonian of the quantum antiferromagnet in the spin wave approximation. Applying the Bogoluibov transformation (2.17): $a_{\mathbf{k}} = \cosh\theta_{\mathbf{k}} \alpha_{\mathbf{k}} - \sinh\theta_{\mathbf{k}} \alpha^\dagger_{-\mathbf{k}}$, etc., with (exercise)

$$\sinh^2\theta_{\mathbf{k}} = \frac{1}{2}\left(\frac{\epsilon^{(0)}_{\mathbf{k}} + Vn}{\epsilon_{\mathbf{k}}} - 1 \right),$$

where $\epsilon_{\mathbf{k}} = [(\epsilon^{(0)}_{\mathbf{k}} + Vn)^2 - (Vn)^2]^{1/2}$, one obtains

$$\hat{H} = \frac{VnN}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0} (\epsilon^{(0)}_{\mathbf{k}} + nV - \epsilon_{\mathbf{k}}) + \sum_{\mathbf{k}\neq 0} \epsilon_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}}.$$

[10] Note that the commutator $[a_0, a_0^\dagger] = 1$ is small as compared to a_0 and $a_0^\dagger$ allowing the field operators to be replaced by the ordinary c-number $\sqrt{N_0}$.

[11] Note that the contact nature of the interaction disguises the presence of the direct and exchange contributions.

From this result, we find that the spectrum of low energy excitations scales linearly as $\epsilon_{\mathbf{k}} \simeq \hbar c|\mathbf{k}|$ where the velocity is given by $c = (Vn/m)^{1/2}$ while, at high energies (when $k \sim k_0 = mc/\hbar$), the spectrum becomes free particle-like.[12]

▷ INFO. Since the number operator $\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}}$ can assume only positive values, one can infer the ground state wavefunction from the condition $\alpha_{\mathbf{k}}|\text{g.s.}\rangle = 0$. Noting that the Bogoliubov transformation can be written as $\alpha_{\mathbf{k}} = Ua_{\mathbf{k}}U^{-1}$, with $U = \exp[\sum_{\mathbf{k}\neq 0} \frac{\theta_{\mathbf{k}}}{2}(a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}} - a_{\mathbf{k}}a_{-\mathbf{k}})]$ (exercise), one can obtain the ground state as $|\text{g.s.}\rangle = U|\Phi\rangle$, where $|\Phi\rangle = (a^\dagger_{\mathbf{k}=0})^N|\Omega\rangle$ denotes the ground state of the ideal Bose gas and $|\Omega\rangle$ the vacuum. The proof follows as

$$0 = a_{\mathbf{k}\neq 0}|\Phi\rangle = U^{-1}\overbrace{Ua_{\mathbf{k}}U^{-1}}^{\alpha_{\mathbf{k}}}U|\Phi\rangle.$$

For the contact interaction, the corresponding ground state energy diverges and must be 'regularised'.[13] In doing so, one obtains $E_0 = \frac{VnN}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon^{(0)}_{\mathbf{k}} + nV - \epsilon_{\mathbf{k}} - \frac{(nV)^2}{2\epsilon^{(0)}_{\mathbf{k}}})$ which, when summed over $\mathbf{k}$, translates to the energy density

$$\frac{E_0}{L^d} = \frac{n^2V}{2}\left[1 + \frac{128}{15\sqrt{\pi}}(na^3)^{1/2}\right],$$

where $a \simeq (m/4\pi\hbar^2)V$ denotes the scattering length of the interaction.

Finally, one may estimate the depletion of the condensate due to interaction.

$$\frac{N - N_0}{N} = \frac{1}{N}\sum_{\mathbf{k}\neq 0}\langle\text{g.s.}|a^\dagger_{\mathbf{k}}a_{\mathbf{k}}|\text{g.s.}\rangle = \frac{1}{N}\sum_{\mathbf{k}\neq 0}\sinh^2\theta_{\mathbf{k}} = \frac{1}{n}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\sinh^2\theta_{\mathbf{k}} = \frac{1}{3\pi^2 n}k_0^3,$$

i.e. ca. one particle per "coherence length" $\xi \sim 1/k_0$. Recast using the scattering length, one obtains

$$\frac{N - N_0}{N} = \frac{8}{3\sqrt{\pi}}(na^3)^{1/2}.$$

How do these prediction compare with experiment?[14] When cooled to temperatures below $4K$, ^{4}He condenses from a gas into a liquid. The ^{4}He atoms obey Bose statistics and, on cooling still further, the liquid undergoes a transition to a superfluid phase in which a fraction of the Helium atoms undergo Bose-Einstein condensation. Within this phase, neutron scattering can be used to probe the elementary excitations of the system. Fig. 2.11 shows the excitation spectrum below the transition temperature. As predicted by the Bogoluibov theory, the spectrum of low-energy excitations is linear. The data also show the limitations of the weakly interacting theory. In Helium, the steric interactions are strong. At higher energy scales an important second branch of excitations known as rotons appear. The latter lie outside the simple hydrodynamic scheme described above.

[12] Physically, the effect of the interaction is to displace particles from the condensate even at $T = 0$.

[13] For details see, e.g., Ref. [1].

[14] For a review of the history of Bose-Einstein condensation see, e.g. Griffin, cond-mat/9901123

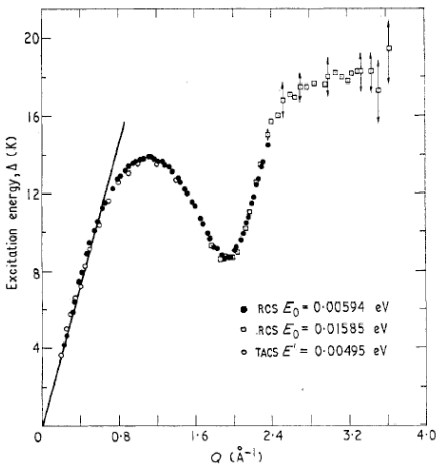


Figure 2.11: The dispersion curve for ^{4}He for the elementary excitations at 1.1K (from Cowley and Woods 1971).

While studies of ^{4}He allow only for the indirect manifestations of Bose-Einstein condensation (viz. superfluidity and elementary excitations of the condensate), recent investigations of dilute atomic gases allow momentum distributions to be explored directly. Following a remarkable sequence of technological breakthroughs in the 90s, dilute vapours of alkali atoms, confined in magnetic traps, were cooled down to extremely low temperatures, of the order of fractions of microkelvins! Here the atoms in the vapour behave as quantum particles obeying Bose or Fermi statistics depending on the atomic number. By abruptly removing the trap, time-of-flight measurements allow the momentum distribution to be inferred directly (see Fig. 2.12a). Below a certain critical temperature, these measurements revealed the development of a sharp peak at low momenta in Bose gases providing a clear signature of Bose-Einstein condensation.

Steven Chu 1948-, **Claude Cohen-Tannoudji** 1933- and **William D. Phillips** 1948-: 1997 Nobel Laureates in Physics for development of methods to cool and trap atoms with laser light.

In the condensed phase, one may measure the sound wave velocity by effecting a density fluctuation using the optical dipole force created by a focused, blue-detuned laser beam. By measuring the speed of propagation of the density fluctuation, the sound wave velocity can be inferred. The latter, shown in Fig. 2.12b, shows a good agreement with the theoretical prediction of the Bogoliubov theory.

2.3 Summary

This concludes our discussion of the second quantisation and its applications to problems in many-body quantum mechanics. Beyond qualitative discussions, the list of applications encountered in this chapter involved problems that were either non–interacting from the outset, or could be reduced to a quadratic operator structure by a number of suitable manipulations. However, we carefully avoided dealing with interacting problems where

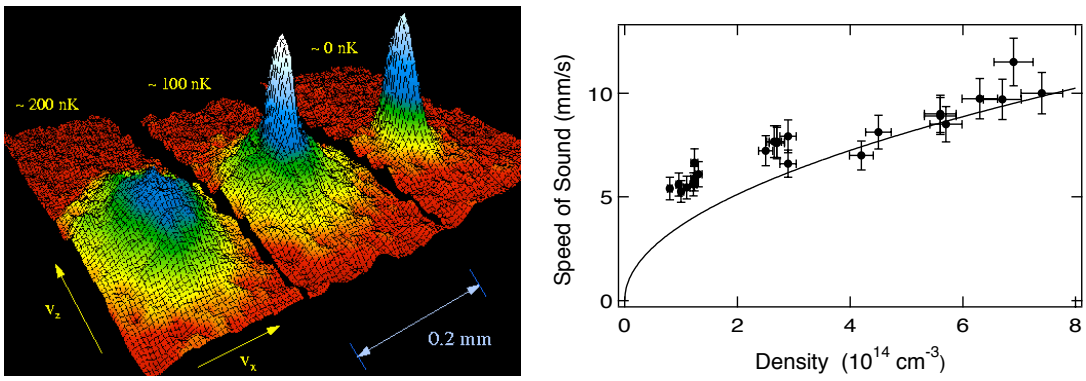


Figure 2.12: Images of the velocity distribution of rubidium atoms by Anderson *et al.* (1995), taken by means of the expansion method. The left frame corresponds to a gas at a temperature just above condensation; the center frame, just after the appearance of the condensate; the right frame, after further evaporation leaves a sample of nearly pure condensate. The field of view is $200\mu\text{m} \times 200\mu\text{m}$, and corresponds to the distance the atoms have moved in about 1/20s. Speed of sound, c vs. condensate peak density N_0 for waves propagating along the axial direction in the condensate. Data taken from Kurn *et al.* (1997) compared to theoretical prediction $c \sim N_0^{1/2}$.

no such reductions are possible. Yet it should be clear already at this stage of our discussion that completely or nearly solvable systems represent only a small minority of the systems encountered in condensed matter physics. What can be done in situations where interactions, i.e. operator contributions of fourth or higher order, are present?

Generically, interacting problems of many-body physics are either fundamentally inaccessible to perturbation theory, or they necessitate perturbative analyses of *infinite* order in the interaction contribution. Situations where a satisfactory result can be obtained by first or second order perturbation theory are exceptional. Within second quantisation, large order perturbative expansions in interaction operators leads to complex polynomials of creation and annihilation operators. Quantum expectation values taken over such structures can be computed by a reductive algorithm, known as **Wick's theorem**. However, from a modern perspective, the formulation of perturbation theory in this way is not very efficient. More importantly, problems that are principally non-perturbative have emerged as a focus of interest. To understand the language of modern quantum condensed matter, we thus need to develop another layer of theory, known as **field integration**. However, before discussing quantum *field* theory, we should understand how the concept works in principle, i.e. on the level of point particle quantum mechanics. This will be the subject of the next chapter.

Chapter 3

Feynman Path Integral

The aim of this chapter is to introduce the concept of the Feynman path integral. As well as developing the general construction scheme, particular emphasis is placed on establishing the interconnections between the quantum mechanical path integral, classical Hamiltonian mechanics and classical statistical mechanics. The practice of path integration is discussed in the context of several pedagogical applications: As well as the canonical examples of a quantum particle in a single and double potential well, we discuss the generalisation of the path integral scheme to tunneling of extended objects (quantum fields), dissipative and thermally assisted quantum tunneling, and the quantum mechanical spin.

In this chapter we will temporarily leave the arena of many–body physics and second quantisation and, at least superficially, return to single–particle quantum mechanics. By establishing the path integral approach for ordinary quantum mechanics, we will set the stage for the introduction of functional field integral methods for many–body theories explored in the next chapter. We will see that the path integral not only represents a gateway to higher dimensional functional integral methods but, when viewed from an appropriate perspective, already represents a field theoretical approach in its own right. Exploiting this connection, various techniques and concepts of field theory, viz. stationary phase analyses of functional integrals, the Euclidean formulation of field theory, instanton techniques, and the role of topological concepts in field theory will be motivated and introduced in this chapter.

3.1 The Path Integral: General Formalism

Broadly speaking, there are two basic approaches to the formulation of quantum mechanics: the 'operator approach' based on the canonical quantisation of physical observables

together with the associated operator algebra, and the Feynman[1] path integral.[2] Whereas canonical quantisation is usually taught first in elementary courses on quantum mechanics, path integrals seem to have acquired the reputation of being a sophisticated concept that is better reserved for advanced courses. Yet this treatment is hardly justified! In fact, the path integral formulation has many advantages most of which explicitly support an intuitive understanding of quantum mechanics. Moreover, integrals — even the infinite dimensional ones encountered below — are hardly more abstract than infinite dimensional linear operators. Further merits of the path integral include the following:

- ▷ Whereas the classical limit is not always easy to retrieve within the canonical formulation of quantum mechanics, it constantly remains visible in the path integral approach. In other words, the path integral makes explicit use of classical mechanics as a basic 'platform' on which to construct a theory of quantum fluctuations. The classical solutions of Hamilton's equation of motion always remain a central ingredient of the formalism.[3]

- ▷ Path integrals allow for an efficient formulation of *non–perturbative* approaches to the solution of quantum mechanical problems. For example, the 'instanton' formulation of quantum tunnelling discussed below — whose extension to continuum theories has led to some of the most powerful concepts of quantum field theory — makes extensive use of the classical equations of motion when it is tailored to a path integral formulation.

- ▷ The Feynman path integral represents a prototype of the higher dimensional functional field integrals to be introduced in the next chapter. However,...

- ▷ ...even in its 'zero–dimensional' form discussed in this chapter, the path integral is of relevance to a wide variety of applications in many–body physics: Very often, one encounters enviroments such as the superconductor, superfluid, or strongly correlated few electron devices where a macroscopically large number of degrees of

[1]

Richard P. Feynman 1918–1988: 1965 Nobel Laureate in Physics (with Sin–Itiro Tomonaga, and Julian Schwinger) for fundamental work in quantum electrodynamics, with deep–ploughing consequences for the physics of elementary particles.

[2]For a more extensive introduction to the Feynman path integral, one can refer to one of the many standard texts including Refs. [9, 16, 20] or, indeed, one may turn to the original paper, R. P. Feynman, *Space–time approach to non–relativistic quantum mechanics*, Rev. Mod. Phys. **20**, 367 (1948). Historically, Feynman's development of the path integral was motivated by earlier work by Dirac on the connection between classical and quantum mechanics, P. A. M. Dirac, *On the analogy between classical and quantum mechanics*, Rev. Mod. Phys. **17**, 195 (1945).

[3]For this reason, path integration has turned out to be an indispensable tool in fields such as **quantum chaos** where the quantum manifestations of classically non–trivial behaviour are investigated — for more details, see section 3.2.2 below.

freedom 'lock' to form a single collective variable. (For example, to a first approximation, the phase information carried by the order parameter field in moderatly large superconducting grains can often be described in terms of a *single* phase degree of freedom, i.e. a 'quantum particle' living on the complex unit circle.) Path integral techniques have proven ideally suited to the analysis of such systems.

What, then, is the basic idea of the path integral approach? More than any other formulation of quantum mechanics, the path integral formalism is based on connections to classical mechanics. The variational approach employed in chapter **??** relied on the fact that classically allowed trajectories in configuration space extremize an action functional. A principal constraint to be imposed on any such trajectory is energy conservation. By contrast, quantum particles have more freedom than their classical counterparts. In particular, by the Uncertainty Principle, energy conservation can be violated by an amount ΔE over a time $\sim \hbar/\Delta E$ (here, and throughout this chapter, we will reinstall $\hbar$ for clarity). The connection to action principles of classical mechanics becomes particularly apparent in problems of quantum tunneling: A particle of energy E may tunnel through a potential barrier of height $V > E$. However, this process is penalized by a damping factor $\sim \exp(i \int_{\text{barrier}} dx\, p/\hbar)$, where $p = \sqrt{2m(E-V)}$, i.e. the exponent of the (imaginary) action associated with the classically forbidden path.

These observations motivate the idea of a new formulation of quantum propagation: Could it be that, as in classical mechanics, the quantum amplitude A for propagation between any two points in coordinate space is again controlled by the action functional? — controlled in a relaxed sense where not just a single extremal path $x_{\text{cl}}(t)$, but an entire manifold of neighbouring paths contribute. More specifically, one might speculate that the quantum amplitude is obtained as $A \sim \sum_{x(t)} \exp(iS[x]/\hbar)$, where $\sum_{x(t)}$ symbolically stands for a summation over all paths compatible with the initial conditions of the problem, and S denotes the *classical* action. Although, at this stage, no formal justification for the path integral has been presented, with this *ansatz*, some features of quantum mechanics would obviously be born out correctly: Specifically, in the classical limit ($\hbar \to 0$), the quantum mechanical amplitude would become increasingly dominated by the contribution to the sum from the classical path $x_{\text{cl}}(t)$. This is because non–extremal configurations would be weighted by a rapidly oscillating amplitude associated with the large phase $S/\hbar$ and would, therefore, average to zero.[4] Secondly, quantum mechanical tunneling would be a natural element of the theory; non–classical paths do contribute to the net–amplitude, but at the cost of a damping factor specified by the imaginary action (as in the traditional formulation).

Fortunately, no fundamentally novel 'picture' of quantum mechanics needs to be declared to promote the idea of the path 'integral' $\sum_{x(t)} \exp(iS[x]/\hbar)$ to a working theory. As we will see in the next section, the new formulation can quantitatively be developed from the same principles of canonical quantization.

[4]More precisely, in the limit of small $\hbar$, the path sum can be evaluated by saddle–point methods, as detailed below.

3.2 Construction of the Path Integral

All information about any autonomous[5] quantum mechanical system is contained in the matrix elements of its time evolution operator. A formal integration of the time–dependent Schrödinger equation $i\hbar\partial_t|\Psi\rangle = \hat{H}|\Psi\rangle$ obtains the time evolution operator

$$|\Psi(t')\rangle = \hat{U}(t',t)|\Psi(t)\rangle, \qquad \hat{U}(t',t) = e^{-\frac{i}{\hbar}\hat{H}(t'-t)}\Theta(t'-t)\,. \tag{3.1}$$

The operator $\hat{U}(t',t)$ describes dynamical evolution under the influence of the Hamiltonian from a time t to time t'. Causality implies that $t' > t$ as indicated by the step or Heaviside Θ–function. In the real space representation we can write

$$\Psi(q',t') = \langle q'|\Psi(t')\rangle = \langle q'|\hat{U}(t',t)\Psi(t)\rangle = \int dq\; U(q',t';q,t)\Psi(q,t)\,,$$

where $U(q',t';q,t) = \langle q'|e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|q\rangle\Theta(t'-t)$ defines the (q',q) component of the time evolution operator. As the matrix element expresses the probability amplitude for a particle to propagate between points q and q' in a time $t'-t$, it is sometimes known as the **propagator** of the theory.

The basic idea behind Feynman's path integral approach is easy to formulate. Rather than attacking the Schrödinger equation governing the time evolution for general times t, one may first attempt to solve the much simpler problem of describing the time evolution for infinitesimally small times Δt. In order to formulate this idea quantitatively one must first 'divide' the time evolution operator into $N \gg 1$ discrete 'time steps',

$$e^{-i\hat{H}t/\hbar} = \left[e^{-i\hat{H}\Delta t/\hbar}\right]^N, \tag{3.2}$$

where $\Delta t = t/N$. Albeit nothing more than a formal rewriting of Eq. (3.1), the representation (3.2) has the advantage that the factors $e^{-i\hat{H}\Delta t/\hbar}$ (or, rather, their expectation values) are small. (More precisely, if Δt is much smaller than the (reciprocal of the) eigenvalues of the Hamiltonian in the regime of physical interest, the exponents are small in comparison with unity and, as such, can be treated perturbatively.) A first simplification arising from this fact is that the exponentials can be factorised into two pieces each of which can be readily diagonalised. To achieve this factorisation, we make use of the identity

$$e^{-i\hat{H}\Delta t/\hbar} = e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar} + O(\Delta t^2)\,,$$

where the Hamiltonian $\hat{H} = \hat{T} + \hat{V}$ is the sum of a kinetic energy $\hat{T} = \hat{p}^2/2m$, and some potential energy operator $\hat{V}$.[6] (The following analysis, restricted for simplicity to a one–dimensional Hamiltonian, is easily generalised to arbitrary spatial dimension.) The key

[5] A system is classified as **autonomous** if its Hamiltonian does not explicitly depend on time. Actually the construction of the path integral can be straightforwardly extended so as to include time–dependent problems. However, in order to keep the introductory discussion as simple as possible, here we assume time–independence.

[6] Although this *ansatz* already covers a wide class of quantum mechanical problems, many applications of practical importance (e.g. Hamiltonians involving spin or magnetic fields) do not fit into this framework. For a detailed exposition covering its realm of applicability, we refer to the specialist literature such as, e.g., Schulman's text [20].

advantage of this factorisation is that the eigenstates of each of the factors $e^{-i\hat{T}\Delta t/\hbar}$ and $e^{-i\hat{V}\Delta t/\hbar}$ are known independently. To exploit this fact we consider the time evolution operator factorised as a product,

$$\langle q_F|\left[e^{-i\hat{H}\Delta t/\hbar}\right]^N|q_I\rangle \simeq \langle q_F|_\wedge e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar}{}_\wedge\cdots{}_\wedge e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar}|q_I\rangle \tag{3.3}$$

and insert at each of the positions indicated by the symbol '$\wedge$' the resolution of identity

$$\text{id.} = \int dq_n \int dp_n |q_n\rangle\langle q_n|p_n\rangle\langle p_n| \,. \tag{3.4}$$

Here $|q_n\rangle$ and $|p_n\rangle$ represent a complete set of position and momentum eigenstates respectively, and $n = 1, \ldots, N$ serves as an index keeping track of the time steps at which the unit operator is inserted. The rational behind the particular choice (3.4) is clear. The unit operator is arranged in such a way that both $\hat{T}$ and $\hat{V}$ act on the corresponding eigenstates. Inserting (3.4) into (3.3), and making use of the identity $\langle q|p\rangle = \langle p|q\rangle^* = e^{iqp/\hbar}/(2\pi\hbar)$, one obtains

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle \simeq \int\limits_{q_N=q_F, q_0=q_I} \prod_{n=1}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} e^{-i\frac{\Delta t}{\hbar}\sum_{n=0}^{N-1}\left(V(q_n)+T(p_{n+1})-p_{n+1}\frac{q_{n+1}-q_n}{\Delta t}\right)} \,. \tag{3.5}$$

Thus, the matrix element of the time evolution operator has been expressed as a $2N-1$ dimensional integral over eigenvalues. Up to corrections of higher order in $V\Delta t/\hbar$ and $T\Delta t/\hbar$, the expression (3.5) is exact. At each 'time step' $t_n = n\Delta t$, $n = 1, \ldots, N$ we are integrating over a pair of coordinates $x_n \equiv (q_n, p_n)$ parametrising the **classical phase space**. Taken together, the points $\{x_n\}$ form an N–point discretization of a path in this space (see Fig. 3.1).

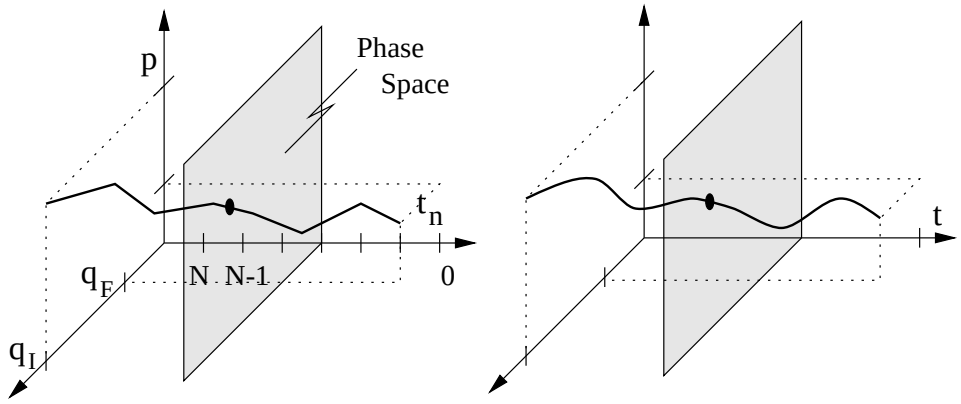


Figure 3.1: Left: visualisation of a set of phase space points contributing to the discrete time configuration integral (3.5). Right: in the continuum limit, the set of points becomes a smooth curve.

To make further progress, we need to develop some intuition for the behaviour of the integral (3.5). We first notice that rapid fluctuations of the integration arguments x_n as

a function of the index n are strongly inhibited by the structure of the integrand. When taken together, contributions for which $(q_{n+1}-q_n)p_{n+1} > O(\hbar)$ (i.e. when the phase of the exponential exceeds 2π) tend to lead to a 'random phase cancellation'. In the language of wave mechanics, the 'incoherent' superposition of different Feynman paths destructively interferes. The *smooth* variation of the paths which contribute significantly motivate the application of a continuum limit analogous to that employed in chapter **??**.

To be specific, sending $N \to \infty$ whilst keeping $t = N\Delta t$ fixed, the formerly discrete set $t_n = n\Delta t,\ n = 1, \ldots, N$ becomes dense on the time interval $[0, t]$, and the set of phase space points $\{x_n\}$ becomes a continuous curve $x(t)$. In the same limit,

$$\Delta t \sum_{n=0}^{N-1} \mapsto \int_0^t dt', \qquad \frac{q_{n+1} - q_n}{\Delta t} \mapsto \partial_{t'} q\Big|_{t'=t_n} \equiv \dot{q}|_{t'=t_n} ,$$

while $[V(q_n) + T(p_{n+1})] \mapsto [T(p|_{t'=t_n}) + V(q|_{t'=t_n})] \equiv H(x|_{t'=t_n})$ denotes the *classical* Hamiltonian. In the limit $N \to \infty$, the fact that kinetic and potential energies are evaluated at neighbouring time slices, n and $n+1$, becomes irrelevant.[7] Finally,

$$\lim_{N\to\infty} \int \prod_{\substack{n=1 \\ q_N = q_F, q_0 = q_I}}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \equiv \int_{\substack{q(t)=q_F \\ q(0)=q_I}} Dx$$

defines the integration measure of the integral.

▷ INFO. Integrals extending over infinite dimensional integration measures like $D(q,p)$ are generally called **functional integrals** (recall our discussion of functionals in chapter **??**). The question of how functional integration can be rigorously defined is far from innocent and represents a subject of current, and partly controversial mathematical research. In this book — as in most applications in physics — we take a pragmatic point of view and deal with the infinite dimensional integration naively unless mathematical problems arise (which actually won't be the case!).

Then, applying these conventions to Eq. (3.5), one finally obtains

$$\boxed{\langle q_F | e^{-i\hat{H}t/\hbar} | q_I \rangle = \int_{\substack{q(t)=q_F \\ q(0)=q_I}} Dx \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(p\dot{q} - H(p,q)\right)\right]} \tag{3.6}$$

[7] To see this formally, one may Taylor expand $T(p_{n+1}) = T(p(t'+\Delta t))|_{t'=n\Delta t}$ around $p(t')$. For smooth $p(t')$, all but the zeroth order contribution $T(p(t'))$, scale with powers of Δt, thereby becoming irrelevant. Note, however, that all of these arguments are based on the assertion that the dominant contributions to the path integral are smooth in the sense $q_{n+1} - q_n \sim O(\Delta t)$. A closer inspection, however, shows that in fact $q_{n+1} - q_n \sim O(\sqrt{\Delta t})$ [20]. In some cases, the most prominent one being the quantum mechanics of a particle in a magnetic field, the lowered power of Δt spoils the naive form of the continuity argument above, and more care must be applied in taking the continuum limit. In cases where a 'new' path integral description of a quantum mechanical problem is developed, it is imperative to delay taking the continuum limit until the fluctuation behaviour of the discrete integral across individual time slices has been thoroughly examined.

Eq. (3.6) represents the **Hamiltonian formulation of the path integral**: The integration extends over all possible paths through the classical phase space of the system which begin and end at the same *configuration* points q_I and q_F respectively (cf. Fig. 3.1). The contribution of each path is weighted by its Hamiltonian action.

Before we turn to the discussion of the path integral (3.6), it is first useful to recast the integral in an alternative form which will be both convenient in various applications and physically instructive. The search for an alternative formulation is motivated by the observation of the close resemblance of (3.6) with the Hamiltonian formulation of classical mechanics. Given that, classically, Hamiltonian and *Lagrangian* mechanics can be equally employed to describe dynamical evolution, it is natural to seek a Lagrangian analogue of (3.6). Until now, we have made no assumption about the momentum dependence of the kinetic energy $T(p)$. However, if we focus on Hamiltonians in which the dynamics is free, i.e. the kinetic energy dependence is quadratic in p, the Lagrangian form of the path integral can be inferred from (3.6) by Gaussian integration.

To make this point clear, let us rewrite the integral in a way that emphasises its dependence on the momentum variable p:

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{\substack{q(t)=q_F\\q(0)=q_I}} Dq\; e^{-\frac{i}{\hbar}\int_0^t dt' V(q)} \int Dp\; e^{-\frac{i}{\hbar}\int_0^t dt'\left(\frac{p^2}{2m}-p\dot{q}\right)}. \tag{3.7}$$

The exponent of the integral is quadratic in the momentum variable or, equivalently, the integral is Gaussian in p. Carrying out the integration by means of Eq. (3.13) below, one obtains

$$\boxed{\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{\substack{q(t)=q_F\\q(0)=q_I}} Dq\; \exp\left[\frac{i}{\hbar}\int_0^t dt' L(q,\dot{q})\right]} \tag{3.8}$$

where $Dq = \lim_{N\to\infty}(\frac{Nm}{it2\pi\hbar})^{N/2}\prod_{n=1}^{N-1} dq_n$ denotes the functional measure of the remaining q–integration, and $L(q,\dot{q}) = m\dot{q}^2/2 - V(q)$ represents the classical Lagrangian. Strictly speaking, the (finite–dimensional) integral formula (3.13) is not directly applicable to the infinite dimensional Gaussian integral (3.7). This, however, does not represent a substantial problem as we can always rediscretise the integral (3.7), apply Eq. (3.13), and reinstate the continuum limit after integration (exercise).

Together Eqs. (3.6) and (3.8) represent the central results of this section. A quantum mechanical transition amplitude has been expressed in terms of an infinite dimensional integral extending over paths through phase space (3.6) or coordinate space (3.8). All paths begin (end) at the initial (final) coordinate of the matrix element. Each path is weighted by its *classical* action. Notice in particular that the quantum transition amplitude has been cast in a form which does not contain quantum mechanical operators. Nonetheless, quantum mechanics is still fully present! The point is that the integration extends over *all* paths and not just the subset of solutions of the classical equations of motion. (The distinguished role classical paths play in the path integral will be discussed below in section 3.2.2.) The two forms of the path integral, (3.6) and (3.8), represent the formal implementation of the 'alternative picture' of quantum mechanics proposed heuristically at the beginning of the chapter.

▷ INFO. **Gaussian Integration**: Apart from a few rare exceptions, all integrals encountered in this course will be of Gaussian[8] form. In most cases the dimension of the integrals will be large if not infinite. Yet, after a bit of practice, it will become clear that high dimensional representatives of Gaussian integrals are no more difficult to handle than their one–dimensional counterparts. Therefore, considering the important role played by Gaussian integration in field theory, we will here derive the principle formulae once and for all. Our starting point is the one–dimensional integral (both real and complex). The basic ideas underlying the proofs of the one–dimensional formulae, will provide the key to the derivation of more complex, multi–dimensional and functional identities which will be used liberally throughout the remainder of the text.

One–dimensional Gaussian integral: The basic ancestor of all Gaussian integrals is the identity

$$\boxed{\int_{-\infty}^{\infty} dx\, e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}, \qquad \text{Re } a > 0} \tag{3.9}$$

In the following we will need various generalisations of Eq. (3.9). Firstly, we have $\int_{-\infty}^{\infty} dx\, e^{-ax^2/2}x^2 = \sqrt{2\pi/a^3}$, a result established either by substituting $a \to a + \epsilon$ in Eq. (3.9) and expanding both the left and the right side of the equation to leading order in ϵ, or by differentiating Eq. (3.9). Often one encounters integrals where the exponent is not purely quadratic from the outset but rather contains both quadratic and linear pieces. The generalisation of Eq. (3.9) to this case reads

$$\int_{-\infty}^{\infty} dx\, e^{-\frac{a}{2}x^2+bx} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}\,. \tag{3.10}$$

To prove this identity, one simply eliminates the linear term by means of the change of variables $x \to x + b/a$ which transforms the exponent to $ax^2/2 + bx \to -ax^2/2 + b^2/2a$. The constant factor scales out and we are left with Eq. (3.9). Note that Eq. (3.10) holds even for complex b. The reason is that by shifting the integration contour into the complex plane no singularities are encountered, i.e. the integral remains invariant.

Later, we will be concerned with the generalisation of the Gaussian integral to complex arguments. In this case, the extension of Eq. (3.9) reads

$$\int d(\bar{z}, z) e^{-\bar{z}wz} = \frac{\pi}{w}, \qquad \text{Re } w > 0\,,$$

where $\bar{z}$ represents the complex conjugate of z. Here, $\int d(\bar{z}, z) \equiv \int_{-\infty}^{\infty} dxdy$ represents the independent integration over the real and imaginary parts of $z = x + iy$. The identity is easy to prove: Owing to the fact that $\bar{z}z = x^2 + y^2$, the integral factorizes into two pieces each of which is equivalent to Eq. (3.9) with $a = w$. Similarly, it may be checked that the complex

8

Johann Carl Friedrich Gauss 1777-1855: worked in a wide variety of fields in both mathematics and physics incuding number theory, analysis, differential geometry, geodesy, magnetism, astronomy and optics. Portrait taken from the former German 10–Mark note. (Unfortunately, the subsequently introduced Euro notes no longer display Gauss' portrait.)

generalisation of Eq. (3.10) is given by

$$\int d(\bar{z},z)e^{-\bar{z}wz+\bar{u}z+\bar{z}v}=\frac{\pi}{w}e^{\frac{\bar{u}v}{w}},\qquad \mathrm{Re}\,w>0\,. \tag{3.11}$$

More importantly $\bar{u}$ and v may be *independent* complex numbers; they need not be related to each other by complex conjugation (exercise).

Gaussian integration in more than one dimension: All of the integrals above have higher dimensional counterparts. Although the real and complex versions of the N–dimensional integral formulae can be derived in a perfectly analogous manner, it is better to discuss them seperately in order not to confuse the notation.

(a) Real Case: The multi–dimensional generalisation of the prototype integral (3.9) reads

$$\int d\mathbf{v}e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}}=(2\pi)^{N/2}\det\mathbf{A}^{-1/2}\,, \tag{3.12}$$

where $\mathbf{A}$ is a positive definite real symmetric N–dimensional matrix and $\mathbf{v}$ is an N–component real vector. The proof makes use of the fact that $\mathbf{A}$ (by virtue of being symmetric) can be diagonalised by orthogonal transformation, $\mathbf{A}=\mathbf{O}^T\mathbf{D}\mathbf{O}$, where the matrix $\mathbf{O}$ is orthogonal, and all elements of the diagonal matrix $\mathbf{D}$ are positive. The matrix $\mathbf{O}$ can be absorbed into the integration vector by means of the variable transformation, $\mathbf{v}\mapsto\mathbf{O}\mathbf{v}$ which has unit Jacobian, $\det\mathbf{O}=1$. As a result, we are left with a Gaussian integral with exponent $-\mathbf{v}^T\mathbf{D}\mathbf{v}/2$. Due to the diagonality of $\mathbf{D}$, the integral factorizes into N independent Gaussian integrals each of which contributes a factor $\sqrt{2\pi/d_i}$, where $d_i,\ i=1,\ldots,N$ is the ith entry of the matrix $\mathbf{D}$. Noting that $\prod_{i=1}^N d_i=\det\mathbf{D}=\det\mathbf{A}$, (3.12) is derived.

The multi–dimensional generalization of (3.10) reads

$$\int d\mathbf{v}e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}+\mathbf{j}^T\cdot\mathbf{v}}=(2\pi)^{N/2}\det\mathbf{A}^{-1/2}e^{\frac{1}{2}\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}} \tag{3.13}$$

where $\mathbf{j}$ is an arbitrary N–component vector. Eq. (3.13) is proven by analogy with Eq. (3.10), i.e. by shifting the integration vector according to $\mathbf{v}\to\mathbf{v}+\mathbf{A}^{-1}\mathbf{j}$, which does not change the value of the integral but removes the linear term from the exponent, $-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}+\mathbf{j}^T\cdot\mathbf{v}\to-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}+\frac{1}{2}\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}$. The resulting integral is of the type (3.12), and we arrive at Eq. (3.13).

The integral (3.13) is not only of importance in its own right, but it also serves as a 'generator' of other useful integral identities. Applying the differentiation operation $\partial^2_{j_mj_n}|_{\mathbf{j}=0}$ to the left and the right hand side of Eq. (3.13), one obtains the identity[9] $\int d\mathbf{v}e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}}v_mv_n=(2\pi)^{N/2}\det\mathbf{A}^{-1/2}A^{-1}_{mn}$. This result can be more compactly formulated as

$$\langle v_mv_n\rangle=A^{-1}_{mn}, \tag{3.14}$$

where we have introduced the shorthand notation

$$\langle\ldots\rangle\equiv(2\pi)^{-N/2}\det\mathbf{A}^{1/2}\int d\mathbf{v}e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}}(\ldots)\,, \tag{3.15}$$

suggesting an interpretation of the Gaussian weight as a probability distribution.

Indeed, the differentiation operation leading to (3.14) can be iterated: Differentiating four times, one obtains $\langle v_mv_nv_qv_p\rangle=A^{-1}_{mn}A^{-1}_{qp}+A^{-1}_{mq}A^{-1}_{np}+A^{-1}_{mp}A^{-1}_{nq}$. One way of memorising the

[9]Note that the notation A^{-1}_{mn} refers to the mn element of the matrix $\mathbf{A}^{-1}$.

structure of this — important — identity is that the Gaussian 'expectation' value $\langle v_m v_n v_p v_q \rangle$ is given by all 'pairings' of type (3.14) that can be formed from the four components v_m. This rule generalises to expectation values of arbitrary order: $2n$–fold differentiation of (3.13) yields

$$\boxed{\langle v_{i_1} v_{i_2} \dots v_{i_{2n}} \rangle = \sum_{\substack{\text{all possible} \\ \text{pairings of} \{i_1, \dots i_{2n}\}}} A^{-1}_{i_{k_1} i_{k_2}} \dots A^{-1}_{i_{k_{2n-1}} i_{k_{2n}}}} \tag{3.16}$$

This result is the mathematical identity underlying **Wick's theorem** (for real bosonic fields).

(b) Complex Case: The results above are straightforwardly extended to multi–dimensional complex Gaussian integrals. The complex version of Eq. (3.12) is given by

$$\int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v}} = \pi^N \det \mathbf{A}^{-1} \,, \tag{3.17}$$

where $\mathbf{v}$ is a complex N–component vector, $d(\mathbf{v}^\dagger, \mathbf{v}) \equiv \prod_{i=1}^N d\mathrm{Re}\, v_i \, d\mathrm{Im}\, v_i$, and $\mathbf{A}$ is a complex matrix with positive definite Hermitian part. (Remember that every matrix can be decomposed into a Hermitian and an anti–Hermitian component, $\mathbf{A} = \frac{1}{2}(\mathbf{A}+\mathbf{A}^\dagger)+\frac{1}{2}(\mathbf{A}-\mathbf{A}^\dagger)$.) For Hermitian $\mathbf{A}$, the proof of (3.17) is analogous to (3.12), i.e. $\mathbf{A}$ is unitarily diagonalisable, $\mathbf{A} = \mathbf{U}^\dagger \mathbf{A} \mathbf{U}$; the matrices $\mathbf{U}$ can be transformed into $\mathbf{v}$, the resulting integral factorises, etc. For non–Hermitian $\mathbf{A}$ the proof is more elaborate, if unedifying, and we refer to the literature for details. The generalization of Eq. (3.17) to exponents with linear contributions reads

$$\int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v} + \mathbf{w}^\dagger \cdot \mathbf{v} + \mathbf{v}^\dagger \cdot \mathbf{w}'} = \pi^N \det \mathbf{A}^{-1} e^{\mathbf{w}^\dagger \mathbf{A}^{-1} \mathbf{w}'} \tag{3.18}$$

Note that $\mathbf{w}$ and $\mathbf{w}'$ may be *independent* complex vectors. The proof of this identity mirrors that of (3.13), i.e. by effecting the shift $\mathbf{v}^\dagger \to \mathbf{v}^\dagger + \mathbf{w}^\dagger$, $\mathbf{v} \to \mathbf{v} + \mathbf{w}'$.[10] As with Eq. (3.13), Eq. (3.18) may also serve as a generator of related integral identities. Differentiating the integral twice according to $\partial^2_{w_m, w'_n}|_{\mathbf{w}=\mathbf{w}'=0}$ gives

$$\langle \bar{v}_m v_n \rangle = A^{-1}_{nm} \,,$$

where $\langle \cdots \rangle \equiv \pi^{-N} \det \mathbf{A} \int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v}} (\cdots)$. The iteration to more than two derivatives gives $\langle \bar{v}_n \bar{v}_m v_p v_q \rangle = A^{-1}_{pm} A^{-1}_{qn} + A^{-1}_{pn} A^{-1}_{qm}$ and, eventually,

$$\boxed{\langle \bar{v}_{i_1} \bar{v}_{i_2} \dots \bar{v}_{i_n} v_{j_1} v_{j_2} \dots v_{j_n} \rangle = \sum_P A^{-1}_{j_1 i_{P1}} \dots A^{-1}_{j_n i_{Pn}}}$$

where $\sum_P$ represents for the sum over all permutations of N integers.

Gaussian Functional Integration: With this preparation, we are in a position to investigate the main practice of quantum and statistical field theory — the method of Gaussian functional integration. Turning to Eq. (3.13), let us suppose that the components of the vector $\mathbf{v}$ parameterise the weight of a real scalar field on the sites of a one–dimensional lattice. In the continuum limit, the set $\{v_i\}$ translates to a function $v(x)$, and the matrix A_{ij} is replaced by an

[10] For an explanation of why $\mathbf{v}$ and $\mathbf{v}^\dagger$ may be shifted independently of each other, cf. the analyticity remarks made in connection with (3.11).

operator kernel or **propagator** $A(x,x')$. In this limit, the natural generalisation of Eq. (3.13) is

$$\int Dv(x) \exp\left[-\frac{1}{2}\int dx\ dx' v(x)A(x,x')v(x') + \int dx\ j(x)v(x)\right] \propto (\det A)^{-1/2} \exp\left[\frac{1}{2}\int dx\ dx'\ j(x)A^{-1}(x,x')j(x')\right], \tag{3.19}$$

where the inverse kernel $A^{-1}(x,x')$ satisfies the equation

$$\boxed{\int dx'\ A(x,x')A^{-1}(x',x'') = \delta(x-x'')} \tag{3.20}$$

i.e. $A^{-1}(x,x')$ can be interpreted as the **Green function** of the operator $A(x,x')$. The notation $Dv(x)$ is used to denote the measure of the functional integral. Although the constant of proportionality, $(2\pi)^N$ left out of Eq. (3.19) is formally divergent in the thermodynamic limit $N \to \infty$, it does not effect averages that are obtained from derivatives of such integrals. For example, for Gaussian distributed functions, Eq. (3.14) has the generalisation

$$\boxed{\langle v(x)v(x')\rangle = A^{-1}(x,x')}$$

Accordingly, Eq. (3.16) assumes the form

$$\boxed{\langle v(x_1)v(x_2)\dots v(x_{2n})\rangle = \sum_{\substack{\text{all possible}\\ \text{pairings of}\{x_1,\dots x_{2n}\}}} A^{-1}(x_{k_1},x_{k_2})\dots A^{-1}(x_{k_{2n-1}},x_{k_{2n}})} \tag{3.21}$$

The generalization of the other Gaussian averaging formulae discussed above should be obvious.

To make sense of Eq. (3.19) one must interpret the meaning of the determinant, det$A$. When the variables entering the Gaussian integral were discrete, the latter simply represented the determinant of the (real symmetric) matrix. In the present case, one must interpret A as an Hermitian operator having an infinite set of eigenvalues. The determinant simply represents the product over this infinite set (see, e.g., section 3.3.1). This completes our discussion of the method of Gaussian integration. Although, in the following section, we will employ only a few of the integral identities above, later we will have occasion to draw on the properties of the 'field averages'.

Before turning to specific applications of the Feynman path integral, let us stay with the general structure of the formalism and identify two fundamental connections of the path integral to *classical point mechanics* and *classical and quantum statistical mechanics*.

3.2.1 Path Integral and Statistical Mechanics

The path integral reveals a connection between quantum mechanics and classical (and quantum) statistical mechanics whose importance to all areas of field theory and statistical physics can hardly be exaggerated. To reveal this link, let us for a moment forget

about quantum mechanics and consider, by way of an example, a perfectly classical, one–dimensional continuum model describing a 'flexible string'. We assume that our string is held under constant tension, and confined to a 'gutter–like potential' (as shown in Fig. 3.2). For simplicity, we also assume that the mass density of the string is pretty high, so that its fluctuations are 'asymptotically slow' (the kinetic contribution to its energy is negligible). Transverse fluctuations of the string are then penalised by its line tension, and by the external potential.

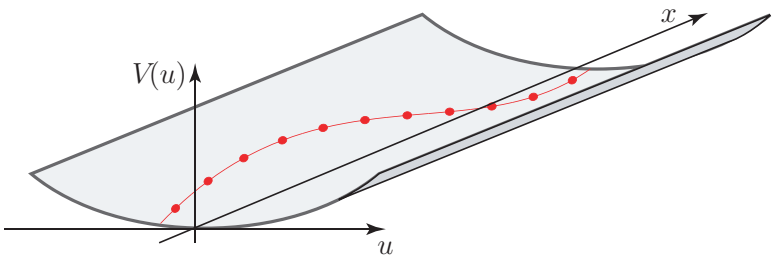


Figure 3.2: A string held under tension and confined to a potential well V.

Assuming that the transverse displacement of the string $u(x)$ is small, the potential energy stored in the string separates into two parts. The first arises form the line tension stored in the string, and the second comes from the external potential. Starting with the former, a transverse fluctuation of a line segment of length dx by an amount du, leads to a potential energy of magnitude $\delta V_{\rm tension} = \sigma[(dx^2+du^2)^{1/2} - -dx] \simeq \sigma dx(\partial_x u)^2/2$, where σ denotes the tension. Integrated over the length of the string, one obtains $V_{\rm tension}[\partial_x u] \equiv \int \delta V_{\rm tension} = \frac{1}{2}\int_0^L dx\ \sigma(\partial_x u(x))^2$. The second contribution arising from the external potential is given by $V_{\rm external}[u] \equiv \int_0^L dx\, V(u(x))$. Adding the two contributions, we find that the total energy of the string is given by $V = V_{\rm tension} + V_{\rm external} = \int_0^L dx[\frac{\sigma}{2}(\partial_x u)^2 + V(u)]$.

According to the general prinicples of statistical mechanics, the equilibrium properties of a system are encoded in the partition function $\mathcal{Z} = {\rm tr}\left[e^{-\beta V}\right]$, where 'tr' denotes a summation over all possible configurations of the system and V is the total potential energy functional. Applied to the present case, ${\rm tr} \to \int Du$, where $\int Du$ stands for the functional integration over all configurations of the string $u(x)$, $x \in [0, L]$. Thus, the partition function of the string is given by

$$\mathcal{Z} = \int Du\ \exp\left[-\beta \int_0^L dx \left(\frac{\sigma}{2}(\partial_x u)^2 + V(u)\right)\right]. \tag{3.22}$$

A comparison of this result with Eq. (3.8) shows that the partition function of the *classical* system coincides with the *quantum mechanical* amplitude

$$\boxed{\mathcal{Z} = \int dq\ \langle q|e^{i\hat{S}[q]/\hbar}|q\rangle\Big|_{t=-iL}}$$

evaluated at an imaginary 'time' $t \to -i\tau \equiv -iL$, where $\hat{H} = \hat{p}^2/2\sigma + V(q)$, and Planck's constant is identified with the 'temperature', $\hbar = 1/\beta$. (Here we have assumed that our string is subject to periodic boundary conditions.)

To see this explicitly, let us assume that we had reason to consider quantum propagation in imaginary time, i.e. $e^{-it\hat{H}/\hbar} \to e^{-\tau\hat{H}/\hbar}$, or $t \to -i\tau$. Assuming convergence (i.e. positivity of the eigenvalues of $\hat{H}$), a construction scheme perfectly analogous to the one outlined in section 3.1 would have led to a path integral formula of the structure (3.8). Formally, the only differece would be that (a) the Lagrangian would be integrated along the imaginary time axis $t' \to -i\tau' \in [0, -i\tau]$ and (b) that there would be a change of the sign of the kinetic energy term, viz. $(\partial_{t'} q)^2 \to -(\partial_{\tau'} q)^2$. After a suitable exchange of variables, $\tau \to L$, $\hbar \to 1/\beta$, the coincidence of the resulting expression with the partition function (3.22) is clear.

The connection between quantum mechanics and classical statistical mechanics outlined above generalises to **higher dimensions**: There are close analogies between quantum field theories in d dimensions and classical statistical mechanics in $d+1$. (The equality of the path integral above with the one–dimensional statistical model is merely the $d = 0$ version of this connection.) In fact, this connection turned out to be one of the major driving forces behind the success of path integral techniques in modern field theory/statistical mechanics. It offered, for the first time, a possibility to draw connections between systems which had seemed unrelated.

However, the concept of imaginary times not only provides a bridge between quantum and classical statistical mechanics, but also plays a role within a purely quantum mechanical context. Consider the *quantum* partition function of a *single particle* quantum mechanical system,

$$\boxed{\mathcal{Z} = \mathrm{tr}[e^{-\beta\hat{H}}] = \int dq\, \langle q|e^{-\beta\hat{H}}|q\rangle}$$

The partition function can be interpreted as a trace over the transition amplitude $\langle q|e^{-i\hat{H}t/\hbar}|q\rangle$ evaluated at an imaginary time $t = -i\hbar\beta$. Thus, real time dynamics and quantum statistical mechanics can be treated on the same footing, provided that we allow for the appearance of imaginary times.

Later we will see that the concept of imaginary or even generalized complex times plays an important role in all of field theory. There is even some nomenclature regarding imaginary times. The transformation $t \to -i\tau$ is denoted as a **Wick rotation** (alluding to the fact that a multiplication with the imaginary unit can be interpreted as a $\pi/2$–rotation in the complex plane). Imaginary time representations of Lagrangian actions are termed **Euclidean**, whereas the real time forms are called **Minkowski**[11] **actions**.

▷ Info. The origin of this terminology can be understood by considering the structure of the action of, say, the phonon model (1.2). Forgetting for a moment about the magnitude of the

[11]

Hermann Minkowski 1864–1909: A pure mathematician credited with the development of a four–dimensional treatment of electrodynamics and, separately, the geometry of numbers.

coupling constants, we see that the action has the bilinear structure $\sim x_\mu g^{\mu\nu} x_\nu$, where $\mu = 0, 1$, the vector $x_\mu = \partial_\mu \phi$ and the diagonal matrix $g = \mathrm{diag}(-1, 1)$ is the two dimensional version of a Minkowski metric. (In three spatial dimensions, g would take the form of the standard Minkowski metric of special relativity.) Wick rotating time, the -1 in the metric changes sign and g becomes a positive definite Euclidean metric. The nature of this transformation motivates the notation above.

Once one has grown accustomed to the idea that the interpretation of time as an imaginary quantity can be useful, yet more general concepts can be conceived. For example, one may contemplate quantum propagation along temporal contours that are neither purely real nor purely imaginary but rather are *generally complex*. Indeed, it has turned out that path integrals with curvelinear integration contours in the complex 'time plane' find numerous applications in statistical and quantum field theory.

3.2.2 Semiclassics from the Path Integral

In deriving the two path integral representations (3.6) and (3.8) no approximations were made. Yet the vast majority of quantum mechanical problems cannot be solved in closed form, and it would be hoping for too much to expect that within the path integral approach this situation would be any different. In fact no more than the path integrals of problems with a quadratic Hamiltonian — corresponding to the quantum mechanical harmonic oscillator and generalisations thereof — can be carried out in closed form. Yet what counts more than the (rare) availability of exact solutions is the flexibility with which *approximation* schemes can be developed. As for the path integral formulation, it is particularly strong in cases where **semiclassical limits of quantum theories** are explored. Here, by 'semiclassical', we mean the limit $\hbar \to 0$, i.e. the case where the theory is expected to be largely governed by classical structures with quantum fluctuations superimposed.

To see more formally how classical structures enter the path integral approach, let us explore Eqs. (3.6) and (3.8) in the limit of small $\hbar$. In this case the path integrals are dominated by path configurations with stationary action. (Non–stationary contributions to the integral imply massive phase fluctuations which largely average to zero.) Now, since the exponents of the two path integrals (3.6) and (3.8) involve the classical action functionals in their Hamiltonian respectively Lagrangian form, the extremal path configurations are simply the solutions of the classical equations of motion, viz.

$$\begin{aligned} \text{Hamiltonian}: \quad & \delta S[x] = 0 \quad \Rightarrow d_t x = \{H(x), x\} \equiv \partial_p H \partial_q x - \partial_q H \partial_p x, \\ \text{Lagrangian}: \quad & \delta S[q] = 0 \quad \Rightarrow (d_t \partial_{\dot q} - \partial_q)\, L(q, \dot q) = 0\,. \end{aligned} \tag{3.23}$$

These equations are to be solved subject to the boundary conditions $q(0) = q_I$ and $q(t) = q_F$. (Note that these boundary conditions do not uniquely specify a solution, i.e. in general there are many solutions to the equations (3.23). As an exercise, one may try to invent examples!)

Now the very fact that the stationary phase configurations are classical does not imply that quantum mechanics has disappeared completely. As with saddle–point approxima-

tions in general, it is not just the saddle–point itself that matters but also the fluctuations around it. At least it is necessary to integrate out Gaussian (quadratic) fluctuations around the point of stationary phase. In the case of the path integral, fluctuations of the action around the stationary phase configurations involve non–classical (in that they do not solve the classical equations of motion) trajectories through phase or coordinate space. Before exploring how this mechanism works in detail, let us consider the stationary phase analysis of functional integrals in general.

▷ Info. **Stationary Phase Approximation**: Consider a general functional integral $\int Dx\, e^{-F[x]}$ where $Dx = \lim_{N\to\infty}\prod_{n=1}^{N} dx_n$ represents a functional measure resulting from taking the continuum limit of some finite dimensional integration space, and the 'action' $F[x]$ may be an arbitrary complex functional of x (leading to convergence of the integral). The function resulting from taking the limit of infinitely many discretisation points, $\{x_n\}$ is denoted by $x : t \mapsto x(t)$ (where t plays the role of the formerly discrete index n). Evaluating the integral above within a stationary phase approximation amounts to performing the following steps:

1. Firstly, find the 'points' of stationary phase, i.e. configurations $\bar{x}$ qualified by the condition of vanishing functional derivative,

$$D_x F = 0 \Leftrightarrow \forall t : \left.\frac{\delta F[x]}{\delta x(t)}\right|_{x=\bar{x}} = 0.$$

   Although there may, in principle, be one or many solutions, for clarity, we first discuss the case in which the stationary phase configuration $\bar{x}$ is unique.

2. Secondly, Taylor expand the functional to second order around $\bar{x}$, viz.

$$F[x] = F[\bar{x}+y] = F[\bar{x}] + \frac{1}{2}\int dt \int dt' y(t') A(t,t') y(t) + \ldots \tag{3.24}$$

   where $A(t,t') = \left.\frac{\delta^2 F[x]}{\delta x(t)\delta x(t')}\right|_{x=\bar{x}}$ denotes the second functional derivative. Due to the stationarity of $\bar{x}$, one may note that no first order contribution can appear.

3. Thirdly, check that the *operator* $\hat{A} \equiv \{A(t,t')\}$ is positive definite. If it is not, there is a problem — the integration over the Gaussian fluctuations y below diverges. (In practice, where the analysis is rooted in a physical context, such eventualities arise only rarely. In situations were problems do occur, the resolution can usually be found in a judicious rotation of the integration contour.) For positive definite $\hat{A}$, however, the functional integral over y can be performed after which one obtains $\int Dx\, e^{-F[x]} \simeq e^{-F[\bar{x}]}\, \det(\frac{\hat{A}}{2\pi})^{-1/2}$, (cf. the discussion of Gaussian integrals above and, in particular, Eq. (3.19)).

4. Finally, if there are many stationary phase configurations, $\bar{x}_i$, the individual contributions have to be added:

$$\int Dx\; e^{-F[x]} \simeq \sum_i e^{-F[\bar{x}_i]}\, \det\left(\frac{\hat{A}_i}{2\pi}\right)^{-1/2}. \tag{3.25}$$

Eq. (3.25) represents the most general form of the stationary phase evaluation of a (real) functional integral.

▷ EXERCISE. Applied to the Gamma function, $\Gamma(z+1) = \int_0^\infty dx\, x^z e^{-x}$, with z complex, show that the stationary phase approximation is consistent with Stirling's approximation, viz. $\Gamma(s+1) = \sqrt{2\pi s} e^{s(\ln s - 1)}$.

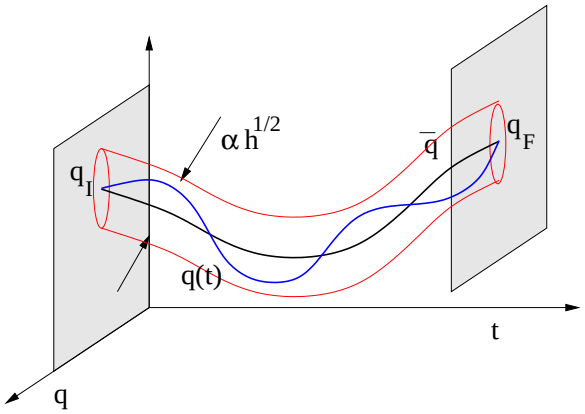


Figure 3.3: Quantum fluctuations around a classical path in coordinate space (here we assume a set of two–dimensional coordinates). Non–classical paths q fluctuating around a classical solution $q_{\rm cl}$ typically extend a distance $O(h^{1/2})$. *All* paths begin and end at q_I and q_F, respectively.

Applied to the Lagrangian form of the Feynman path integral, this program can be implemented directly. In this case, the extremal field configuration $\bar{q}(t)$ is identified as the classical solution associated with the Lagrangian, i.e. $\bar{q}(t) \equiv q_{\rm cl}(t)$. Defining $r(t) = q(t) - q_{\rm cl}(t)$ as the deviation of a general path, $q(t)$, from a nearby classical path, $q_{\rm cl}(t)$ (see Fig. 3.3), and assuming for simplicity that there exists only one classical solution connecting q_I with q_F in a time t, a stationary phase analysis obtains

$$\langle q_F | e^{-i\hat{H}t/\hbar} | q_I \rangle \simeq e^{iS[q_{\rm cl}]/\hbar} \int_{r(0)=r(t)=0} Dr \exp\left[\frac{i}{2\hbar} \int_0^t dt' dt'' r(t') \left. \frac{\delta^2 S[q]}{\delta q(t') \delta q(t'')} \right|_{q=q_{\rm cl}} r(t'') \right] \quad (3.26)$$

as the Gaussian approximation to the path integral (cf. Eq. (3.24)). For free Lagrangians of the form, $L(q,\dot{q}) = m\dot{q}^2/2 - V(q)$, the second functional derivative of the action can be straightforwardly computed by means of the rules of functional differentiation formulated in chapter 1. Alternatively, one can obtain this result by simply expanding the action as a Taylor series in the deviation $r(t)$. As a result, one obtains (exercise)

$$\frac{1}{2} \int_0^t dt \int dt' r(t) \left. \frac{\delta^2 S[q]}{\delta q(t) \delta q(t')} \right|_{q=q_{\rm cl}} r(t') = -\frac{1}{2} \int dt\; r(t) \left[m\partial_t^2 + V''(q_{\rm cl}(t)) \right] r(t)\,, \quad (3.27)$$

where $V''(q_{\rm cl}(t)) \equiv \partial_q^2 V(q)|_{q=q_{\rm cl}}$ represents the ordinary (second) derivative of the potential function evaluated at $q_{\rm cl}(t)$. Thus, the Gaussian integration over r yields the square root of the determinant of the operator $m\partial_t^2 + V''(q_{\rm cl}(t))$ — interpreted as an operator acting in the space of functions $r(t)$ with boundary conditions $r(0) = r(t) = 0$. (Note that, as we are dealing with a differential operator, the issue of boundary conditions is crucial.)

▷ INFO. More generally, Gaussian integration over fluctuations around the stationary phase configuration obtains the formal expression

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle \simeq \det\left(\frac{i}{2\pi\hbar}\frac{\partial^2 S[q_{\rm cl}]}{\partial q_I \partial q_F}\right)^{1/2} e^{\frac{i}{\hbar}S[q_{\rm cl}]}\,, \tag{3.28}$$

as the final result for the **transition amplitude evaluated in the semiclassical approximation**. (In cases where there is more than one classical solution, the individual contributions have to be added.) To derive this expression, one shows that the operator controlling the quadratic action (3.27) fulfills some differential relations which can be, again, related back to the classical action. While a detailed formulation of this calculation (see, for example, Ref. [20], page 94) is beyond the scope of the present text, the heuristic interpretation of the result is straightforward:

According to the rules of quantum mechanics $p(q_F, q_I, t) = |\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle|^2$ defines the probability density for a particle injected at coordinate q_I to arrive at coordinate q_F after a time t. In the semiclassical approximation, the probability density assumes the form $p(q_F, q_I, t) = |\det(\frac{1}{2\pi\hbar}\frac{\partial^2 S[q_{\rm cl}]}{\partial q_I \partial q_F})|$. We can gain some physical insight into this expression from the following consideration: For a fixed inital coordinate q_I, the final coordinate $q_F(q_I, p_I)$ becomes a function of the initial *momentum* p_I. The classical probability density $p(q_I, q_F)$ can then be related to the probabilty density $\tilde{p}(q_I, p_I)$ for a particle to leave from the initial phase space coordinate (q_I, p_I) according to

$$p(q_I, q_F)dq_I dq_F = p(q_I, q_F)\left|\det\left(\frac{\partial q_F}{\partial p_I}\right)\right| dq_I dp_I = \tilde{p}(q_I, p_I)dq_I dp_I.$$

Now, when we say that our particle actually left at the phase space coordinate (q_I, p_I), $\tilde{p}$ becomes singular at (q_I, p_I) while being zero everywhere else. In quantum mechanics, however, all we can say is that our particle was initially confined to a *Planck cell* centered around (q_I, p_I): $\tilde{p}(q_I, p_I) = 1/(2\pi\hbar)^d$. We thus conclude that $p(q_I, q_F) = |\det(\partial p_I/\partial q_F)|\hbar^{-d}$. Finally, noticing that $p_I = -\partial_{q_I} S$ we arrive at the result of the semiclassical analysis above.

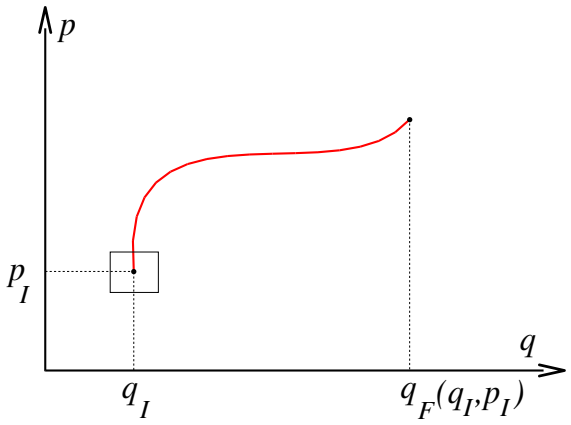


Figure 3.4: Trajectory in two-dimensional phase space: For fixed initial coordinate q_I, the final coordinate $q_F(q_I, p_I)$ becomes a function of the initial momentum. In quantum mechanics, the Planck cell $\hbar^d$ (indicated by the rectangle) limits the accuracy at which the initial coordinate can be set.

In deriving (3.28) we have restricted ourselves to the consideration of *quadratic* fluctuations around the classical paths — the essence of the semiclassical approximation. Under what conditions is this approximation justified? Unfortunately there is no rigorous and generally applicable

answer to this question: For finite $\hbar$, the quality of the approximation depends largely on the sensitivity of the action to path variations. Whether or not the approximation is legitimate is a question that has to be judged from case to case. However, the *asymptotic* stability of the semiclassical approximation in the limit $\hbar \to 0$, can be deduced simply from power counting. From the structure of Eq. (3.28) it is clear that the typical magnitude of fluctuations $r(t)$ scales as $r \sim (\hbar/\delta_q^2 S)^{1/2}$, where $\delta_q^2 S$ is a symbolic shorthand for the functional variation of the action. (Variations larger than that lead to phase fluctuations $> 2\pi$, thereby being negligible.) Non–Gaussian contributions to the action would have the structure $\sim \hbar^{-1} r^n \delta_q^n S$, $n > 2$. For a typical r, this is of the order $\sim \delta_q^n S/(\delta_q^2 S)^{n/2}\hbar^{n/2-1}$. Since the S-dependent factors are classical ($\hbar$–independent), these contributions scale to zero as $\hbar \to 0$.

This concludes the conceptual part of the chapter. Before turning to the discussion of specific applications of the path integral, let us first briefly recapitulate the main steps taken in its construction:

3.2.3 Construction Recipe of the Path Integral

Consider a general quantum transition amplitude $\langle\psi|e^{-i\hat{H}t/\hbar}|\psi'\rangle$, where t may be real, purely imaginary or generally complex. To construct a functional integral representation of the amplitude:

1. Partition the time interval into $N \gg 1$ steps,

$$e^{-i\hat{H}t/\hbar} = \left[e^{-i\hat{H}\Delta t/\hbar}\right]^N, \qquad \Delta t = t/N\,.$$

2. Regroup the operator content appearing in the expansion of each factor $e^{-i\hat{H}\Delta t/\hbar}$ according to the relation

$$e^{-i\hat{H}\Delta t/\hbar} = 1 + \Delta t \sum_{mn} c_{mn}\hat{A}^m\hat{B}^n + O(\Delta t^2)\,,$$

where the eigenstates $|a\rangle, |b\rangle$ of $\hat{A}, \hat{B}$ are known and the coefficients c_{mn} are c–numbers. (In the quantum mechanical application above $\hat{A} = \hat{p}$, $\hat{B} = \hat{q}$.) This 'normal ordering' procedure emphasizes that many distinct quantum mechanical systems are associated with the same classical action.

3. Insert resolutions of identity according to

$$\begin{aligned} e^{-i\hat{H}\Delta t/\hbar} &= \sum_{a,b} |a\rangle\langle a|(1 + \Delta t \sum_{mn} c_{mn}\hat{A}^m\hat{B}^n + O(\Delta t^2))|b\rangle\langle b| \\ &= \sum_{a,b} |a\rangle\langle a|e^{-iH(a,b)\Delta t/\hbar}|b\rangle\langle b| + O(\Delta t^2)\,, \end{aligned}$$

where $H(a,b)$ is the Hamiltonian evaluated at the eigenvalues of $\hat{A}$ and $\hat{B}$.

4. Regroup terms in the exponent: Due to the 'mismatch' of the eigenstates at neighbouring time slices n and $n+1$, not only the Hamiltonians $H(a,b)$, but also sums over differences of eigenvalues appear (cf. the last term in the action (3.5)).

5. Take the continuum limit.

3.3 Applications of the Feynman Path Integral

Having introduced the general machinery of path integration we now turn to the discussion of specific applications. Our starting point will be an investigation of a low energy quantum particle confined to a single potential well, and the phenomenon of tunneling in a double well. With the latter, we will become acquainted with instanton techniques and the role of topology in field theory. The ideas developed in this section will be generalised further to the investigation of quantum mechanical decay and quantum dissipation. Finally, we will turn our attention to the development of the path integral for quantum mechanical spin and, as a case study, explore the semiclassical trace formulae for quantum chaos.

The simplest example of a quantum mechanical problem is that of a **free particle** ($\hat{H} = \hat{p}^2/2m$). Yet, within the framework of the path integral, this example, which can be dealt with straightforwardly by elementary means, is far from trivial: the Gaussian functional integral engaged in its construction involves divergences which must be regularised by rediscretising the path integral. Nevertheless, its knowledge will be useful as a means to normalise the path integral in the applications below. Therefore, we leave it as an exercise to show[12]

$$\boxed{G_{\rm free}(q_F,q_I;t) \equiv \langle q_F|e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t}|q_I\rangle\Theta(t) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2t}(q_F-q_I)^2}\Theta(t)} \tag{3.29}$$

where the Heaviside Θ–function reflects causality.[13]

▷ Exercise. Derive Eq. (3.29) by the standard methodology of quantum mechanics. Hint: insert a resolution of identity and perform a Gaussian integral.

▷ Exercise. Using the path integral, obtain a perturbative expansion for the scattering amplitude $\langle \mathbf{p}'|U(t\to\infty, t'\to-\infty)|\mathbf{p}\rangle$ of a free particle from a short–ranged central potential $V(r)$. In particular, show that the first order term in the expansion recovers the Born scattering amplitude $-i\hbar e^{-i(t-t')E(p)/\hbar}\delta(E(p)-E(p'))\,\langle \mathbf{p}'|V|\mathbf{p}\rangle$.

[12] Compare this result to the solution of a classical diffusion equation.

[13] Motivated by its interpretation as a Green function, in the following we will refer to the quantum transition probability amplitude by the symbol G (as opposed to U used above).

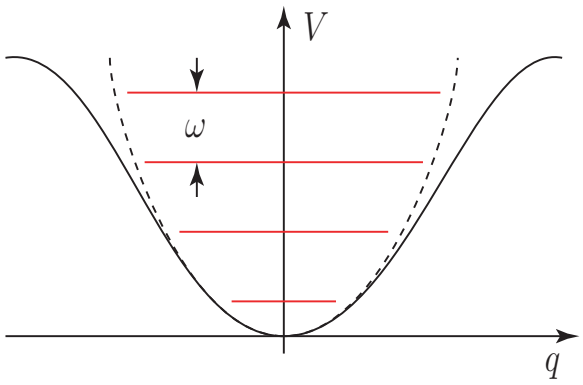


Figure 3.5: Solid: Potential well. Dashed: Quadratic fit approximating the potential shape close to the minimum.

3.3.1 Quantum Particle in a Well

As a first application of the path integral, let us consider the problem of a quantum particle in a one–dimensional potential well (see the figure). The discussion of this example will illustrate how the semiclassical evaluation scheme discussed above works in practice. For simplicity we assume the potential to be symmetric, $V(q) = V(-q)$ with $V(0) = 0$. The quantity we wish to compute is the probability amplitude that a particle injected at $q = 0$ returns after a time t, i.e. with $\hat{H} = \hat{p}^2/2m + V(\hat{q})$, $G(0,0;t) \equiv \langle q_F = 0|e^{-i\hat{H}t/\hbar}|q_I = 0\rangle\Theta(t)$. Drawing on our previous discussion, the path integral representation of the transition amplitude is given by

$$G(0,0;t) = \int_{q(t)=q(0)=0} Dq \exp\left[\frac{i}{\hbar}\int_0^t dt' L(q,\dot{q})\right],$$

where $L = m\dot{q}^2/2 - V(q)$ represents the corresponding Lagrangian.

Now, for a generic potential $V(q)$, the path integral can not be evaluated exactly. Instead, we wish to invoke the semiclassical analysis outlined conceptually above. Accordingly, we must first find solutions to the classical equation of motion. Minimising the action with respect to variations of $q(t)$, one obtains the Euler–Lagrange equation of motion $m\ddot{q} = -V'(q)$ where, as usual, we have used the shorthand $V'(q) \equiv \partial_q V(q)$. According to the Feynman path integral, this equation must be solved subject to the boundary conditions $q(t) = q(0) = 0$. One solution is obvious, viz. $q_{\rm cl}(t) = 0$. Assuming that this is in fact the only solution,[14] we obtain (cf. Eqs. (3.26) and (3.27))

$$G(0,0;t) \simeq \int_{r(0)=r(t)=0} Dr \exp\left[-\frac{i}{\hbar}\int_0^t dt' r(t')\frac{m}{2}\left(\partial_{t'}^2 + \omega^2\right) r(t')\right],$$

[14] In general, this assumption is wrong: For smooth potentials $V(q)$, a Taylor expansion of V at small q obtains the harmonic oscillator potential, $V(q) = V_0 + m\omega^2 q^2/2 + \cdots$. For times t that are commensurate with π/ω, one has periodic solutions, $q_{\rm cl}(t) \propto \sin(\omega t)$ that start out from the origin at time $t = 0$ and revisit it at just the right time t. In the next section we will see why the restriction to just the trivial solution was nonetheless legitimate (for arbitrary times t).

where, by definition, $m\omega^2 \equiv V''(0)$ is the second derivative of the potential at the origin.[15] Note that, in this case, the contribution to the action from the stationary phase field configuration vanishes $S[q_{\rm cl}] = 0$. Following the discussion of section 3.2, Gaussian functional integration over r then leads to the semiclassical expansion

$$G(0,0;t) \simeq J \det\left(-m(\partial_t^2 + \omega^2)/2\right)^{-1/2} , \tag{3.30}$$

where the prefactor J absorbs various constant prefactors.

Operator determinants are usually most conveniently obtained by presenting them as a product over eigenvalues. In the present case, the eigenvalues ϵ_n are determined by the equation

$$-\frac{m}{2}\left(\partial_t^2 + \omega^2\right) r_n = \epsilon_n r_n ,$$

which is to be solved subject to the boundary condition $r_n(t) = r_n(0) = 0$. A complete set of solutions to this equation is given by[16] $r_n(t') = \sin(n\pi t'/t)$, $n = 1, 2, \ldots$, with eigenvalues $\epsilon_n = m[(n\pi/t)^2 - \omega^2]/2$. Applied to the determinant, one therefore finds

$$\det\left(-m(\partial_t^2 + \omega^2)/2\right)^{-1/2} = \prod_{n=1}^{\infty}\left[\frac{m}{2}\left(\left(\frac{n\pi}{t}\right)^2 - \omega^2\right)\right]^{-1/2} .$$

To interpret this result, one must first make sense of the infinite product (which even seems divergent for times commensurate with π/ω!). Moreover the value of the constant J has yet to be properly determined. To resolve these difficulties, one may exploit the fact that (a) we do know the transition amplitude (3.29) of the *free* particle system, and (b) the latter coincides with the transition amplitude G in the special case where the potential $V \equiv 0$. In other words, had we computed $G_{\rm free}$ via the path integral, we would have obtained the same constant J and, more importantly, an infinite product like the one above, but with $\omega = 0$. This allows the transition amplitude to be regularised as

$$G(0,0;t) \equiv \frac{G(0,0;t)}{G_{\rm free}(0,0;t)} G_{\rm free}(0,0;t) = \prod_{n=1}^{\infty}\left[1 - \left(\frac{\omega t}{n\pi}\right)^2\right]^{-1/2} \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \Theta(t) .$$

Then, with the help of the mathematical identity $\prod_{n=1}^{\infty}[1 - (x/n\pi)^2]^{-1} = x/\sin x$, one finally arrives at the result

$$G(0,0;t) \simeq \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega t)}}\,\Theta(t) . \tag{3.31}$$

In the case of the harmonic oscillator, the expansion of the potential necessarily truncates at quadratic order and, in this case, the expression above is exact. (For a more ranging discussion of the path integral for the quantum harmonic oscillator system, see

[15] Those who are uncomfortable with functional differentiation can arrive at the same expression simply by substituting $q(t) = q_{\rm cl}(t) + r(t)$ into the action and expanding in r.

[16] To find the solutions of this equation, recall the structure of the Schrödinger equation of a particle in a one–dimensional box of width $L = t$!

problem 3.5.) For a general potential, the semiclassical approximation effectively involves the replacement of $V(q)$ by a quadratic potential with the same curvature. The calculation above also illustrates how coordinate space fluctuations around a completely static solution may reinstate the zero–point fluctuations characteristic of quantum mechanical bound states.

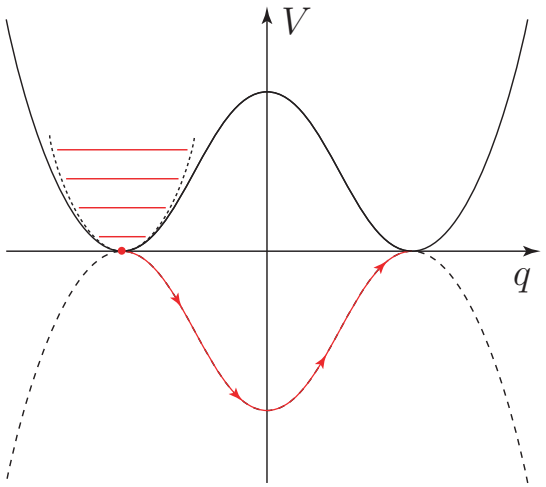


Figure 3.6: Solid: Double well potential. Dashed: Inverted potential

3.3.2 Double Well Potential: Tunneling and Instantons

As a second application of the path integral let us now consider the motion of a particle in a double well potential (see the figure). Our aim will be to estimate the quantum probability amplitude for a particle to either stay at the bottom of one of the local minima *or* to go from one minimum to the other. In doing so, it is understood that the energy range accessible to the particle (i.e. $\Delta E \sim \hbar/t$) is well below the potential barrier height, i.e. quantum mechanical transfer between minima is by *tunnelling*. Here, in contrast to the single well system, it is far from clear what kind of classical stationary phase solutions may serve as a basis for a description of quantum tunnelling; there appear to be no classical paths connecting the two minima. Of course one may think of particles 'rolling' over the potential hill. Yet, these are singular and, by assumption, energetically inaccessible.

The key to resolving these difficulties is an observation, already made above, that the time argument appearing in the path integral should be considered as a general complex quantity that can (according to convenience) be sent to any value in the complex plane. In the present case, a Wick rotation to imaginary times will reveal a stationary point of the action. At the end of the calculation, the *real* time amplitudes we seek can be straightforwardly obtained by analytic continuation.

To be specific, let us consider the imaginary time transition amplitudes

$$G_E(a, \pm a; \tau) \equiv \langle \pm a | \exp\left[-\frac{\tau}{\hbar}\hat{H}\right] |a\rangle = G(-a, \mp a; \tau) \tag{3.32}$$

where the coordinates $\pm a$ coincide with the two minima of the potential. From (3.32) the real time amplitudes $G(a, \pm a; t)$ can be recovered by the analytic continuation $\tau \to it$. According to section 3.2.1, the **Euclidean path integral** formulation of the transition amplitudes is given by

$$\boxed{G(a, \pm a; \tau) = \int_{q(0)=\pm a, q(\tau)=a} Dq \ \exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' \left(\frac{m}{2}\dot{q}^2 + V(q)\right)\right]} \tag{3.33}$$

where the function q now depends on imaginary time. From (3.33) we obtain the stationary phase (or saddle–point) equations

$$-m\ddot{q} + V'(q) = 0. \tag{3.34}$$

From this result, one can infer that, as a consequence of the Wick rotation, there is an effective *inversion* of the potential, $V \to -V$ (shown dashed in the figure above). The crucial point is that, within the inverted potential landscape, the barrier has become a sink, i.e. within the new formulation, there *are* classical solutions connecting the two points, $\pm a$. More precisely, there are three different types of classical solutions which fulfill the condition to be at coordinates $\pm a$ at times 0 and/or τ: (a) The solution wherein the particle rests permanently at a,[17] (b) the corresponding solution staying at $-a$ and, most importantly, (c) the solution in which the particle leaves its initial position at $\pm a$, accelerates through the minimum at 0 and eventually reaches the final position $\mp a$ at time τ. In computing the transition amplitudes, all three types of paths have to be taken into account. As for (a) and (b), by computing quantum fluctuations around these solutions, one can recover the physics of the zero–point motion described in section 3.3.1 for each well individually (exercise: convince yourself that this is true!). Now let us see what happens if the paths connecting the two coordinates are added to this picture.

The Instanton Gas

The classical solution of the Euclidean equation of motion that connects the two potential maxima is called an **instanton solution** while a solution traversing the same path but in the opposite direction ('$-a \to a$' $\rightsquigarrow$ '$a \to -a$') is called an anti–instanton. The name 'instanton' was invented by 't Hooft[18] with the idea that these objects are very similar in

[17] Note that the potential inversion answers a question that arose above, i.e. whether or not the classical solution staying at the bottom of the single well was actually the only one to be considered. As with the double well, we could have treated the single well within an imaginary time representation, whereupon the well would have become a hill. Clearly there is just one classical solution being at two different times at the top of the hill, viz. the solution that stays there forever. By formulating the semiclassical expansion around that path, we would have obtained (3.31) with $t \to -i\tau$, which, upon analytic continuation, would have led back to the real time result.

[18]

Gerardus 't Hooft 1946– : 1999 Nobel Laureate in Physics for elucidating the quantum structure of electroweak interactions in physics.

their mathematical structure to 'solitons', particle–like solutions of classical field theories. However, unlike solitons, they are structures in time (albeit Euclidean time); thus the 'instant–'. As another etymographic remark, note that the syllable '–on' in 'instanton' hints to an interpretation of these states as a kind of particle. The background is that, as a function of the time coordinate, instantons are almost everywhere constant save for a short region of variation (see below). Alluding to the interpretation of time as something akin to a spatial dimension, these states can be interpreted as a well–localised excitation or, according to standard field theoretical practice, a *particle*.[19]

To proceed, we must first compute the classical action associated with a single instanton solution. Multiplying (3.34) by $\dot{q}_{\rm cl}$, integrating over time (i.e. performing the first integral of the equation of motion), and using the fact that at $q_{\rm cl} = \pm a$, $\dot{q}_{\rm cl} = 0$ and $V = 0$, one finds that

$$\frac{m}{2}\dot{q}_{\rm cl}^2 = V(q_{\rm cl}). \tag{3.35}$$

With this result, one obtains the instanton action

$$S_{\rm inst} = \int_0^\tau d\tau' \overbrace{\left(\frac{m}{2}\dot{q}_{\rm cl}^2 + V(q_{\rm cl})\right)}^{m\dot{q}_{\rm cl}^2} = \int d\tau' \, \frac{dq_{\rm cl}}{d\tau'}(m\dot{q}_{\rm cl}) = \int_{-a}^{a} dq \, (2mV(q))^{1/2}. \tag{3.36}$$

Notice that $S_{\rm inst}$ is determined solely by the functional profile of the potential V (i.e. does not depend on the structure of the solution $q_{\rm cl}$).

Secondly, let us explore the structure of the instanton as a function of time. Defining the second derivative of the potential at $\pm a$ by $V''(\pm a) = m\omega^2$, Eq. (3.35) implies that for large times (where the particle is close to the right maximum), $\dot{q}_{\rm cl} = -\omega(q_{\rm cl} - a)$ which integrates to $q_{\rm cl}(\tau) \stackrel{\tau\to\infty}{\longrightarrow} a - e^{-\tau\omega}$. Thus the temporal extension of the instanton is set by the oscillator frequencies of the local potential minima (the maxima of the inverted potential) and, in cases where tunnelling takes place on time scales much larger than that, can be regarded as short (see Fig. 3.7).

The confinement of the instanton configuration to a narrow interval of time has an important implication — there must exist *approximate* solutions of the stationary equation involving further anti–instanton/instanton pairs (physically, the particle repeatedly bouncing to and fro in the inverted potential). According to the general philosophy of the saddle–point scheme, the path integral is obtained by summing over all solutions of the saddle–point equations and hence over all instanton configurations. The summation over multi–instanton configurations — termed the '**instanton gas**' — is substantially simplified by the fact that individual instantons have short temporal support (events of overlapping configurations are rare) and that not too many instantons can be accommodated in a finite time interval (the instanton gas is dilute). The actual density is dictated by the competition between the configurational 'entropy' (favouring high density), and

[19] In addition to the original literature, the importance that has been attached to the instanton method has inspired a variety of excellent and pedagogical reviews of the field. Of these, the following are highly recommended: A. M. Polyakov, *Quark confinement and topology of gauge theories*, Nucl. Phys. **B120**, 429 (1977); S. Coleman, in *Aspects of symmetry — selected Erice lectures*, (Cambridge University Press 1985) chapter 7.

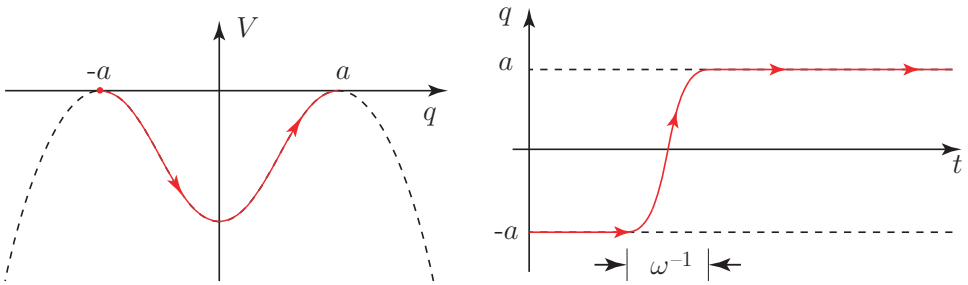


Figure 3.7: Single instanton configuration.

the 'energetics', the exponential weight implied by the action (favouring low density) — see the estimate below.

In practice, multi–instanton configurations imply a transition amplitude

$$G(a,\pm a;\tau) \simeq \sum_{n \text{ even}/\text{odd}} K^n \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n A_n(\tau_1,\ldots,\tau_n), \tag{3.37}$$

where A_n denotes the amplitude associated with n instantons, and we have taken into account the fact that in order to connect a with $\pm a$, the number of instantons must be even/odd. The n instanton bounces contributing to each A_n can take place at arbitrary times $\tau_i \in [0,\tau]$, $i = 1,\ldots,n$ and all these possibilities have to be added (i.e. integrated). Here K denotes a (dimensionful) constant absorbing the temporal dimension $[\text{time}]^n$ introduced by the time integrations, and $A_n(\tau_1,\ldots,\tau_n)$ is the transition amplitude, evaluated within the semiclassical approximation around a configuration of n instanton bounces at times $0 \le \tau_1 < \tau_2 < \ldots < \tau_n \le \tau$ (see Fig. 3.8). In the following, we will first focus on the transition amplitude A_n which controls the exponential dependence of the tunneling amplitude returning later to consider the prefactor K.

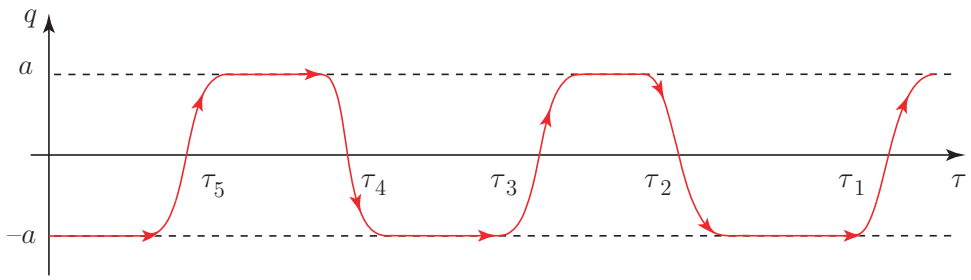


Figure 3.8: Dilute instanton gas configuration.

According to the general semiclassical principle, each amplitude $A_n = A_{n,\text{cl.}} \times A_{n,\text{qu.}}$ factorises into two parts, a classical contribution $A_{n,\text{cl.}}$ accounting for the action of the instanton configuration; and a quantum contribution $A_{n,\text{qu.}}$ resulting from quadratic fluctuations around the classical path. Focusing initially on $A_{n,\text{cl.}}$ we note that, at intermediate times, $\tau_i \ll \tau' \ll \tau_{i+1}$, where the particle rests on top of either of the maxima at $\pm a$,

no action accumulates (cf. the previous section). However, each instanton bounce has a finite action $S_{\rm inst}$ (see Eq. (3.36)) and these contributions add up to give the full classical action,

$$A_{n,\rm cl.}(\tau_1,\ldots,\tau_n) = e^{-nS_{\rm inst}/\hbar}, \tag{3.38}$$

which is independent of the time coordinates τ_i. (The individual instantons 'don't know of each other'; their action is independent of their relative position.)

As for the quantum factor $A_{n,\rm qu.}$, there are, in principle, two contributions. Whilst the particle rests on either of the hills (the straight segments in Fig. 3.8), quadratic fluctuations around the classical (i.e. spatially constant) configuration play the same role as the quantum fluctuations considered in the previous section, the only difference being that we are working in a Wick rotated picture. There it was found that quantum fluctuations around a classical configuration which stays for a (real) time t at the bottom of the well, result in a factor $\sqrt{1/\sin(\omega t)}$ (the remaining constants being absorbed into the prefactor K^n). Rotating to imaginary times, $t \to -i\tau$, one can infer that the quantum fluctuation accumulated during the stationary time $\tau_{i+1} - \tau_i$ is given by

$$\sqrt{\frac{1}{\sin(-i\omega(\tau_{i+1}-\tau_i))}} \sim e^{-\omega(\tau_{i+1}-\tau_i)/2},$$

where we have used the fact that, for the dilute configuration, the typical separation times between bounces are much larger than the inverse of the characteristic oscillator scales of each of the minima. (It takes the particle much longer to tunnel through a high barrier than to oscillate in either of the wells of the *real* potential.)

Now, in principle, there are also fluctuations around the 'bouncing' segments of the path. However, due to the fact that a bounce takes a time of $O(\omega^{-1}) \ll \Delta\tau$, where $\Delta\tau$ represents the typical time *between* bounces, one can neglect these contributions (which is to say that they can be absorbed into the prefactor K without explicit calculation). Within this approximation, setting $\tau_0 \equiv 0$, $\tau_{n+1} \equiv \tau$, the overall quantum fluctuation correction is given by

$$A_{n,\rm qu.}(\tau_1,\ldots,\tau_n) = \prod_{i=0}^{n} e^{-\omega(\tau_{i+1}-\tau_i)/2} = e^{-\omega\tau/2}, \tag{3.39}$$

again independent of the particular spacial configuration $\{\tau_i\}$. Combining (3.38) and (3.39), one finds that

$$\begin{aligned} G(a,\pm a;\tau) &\simeq \sum_{n \text{ even / odd}}^{\infty} K^n e^{-nS_{\rm inst}/\hbar} e^{-\omega\tau/2} \overbrace{\int_0^{\tau} d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n}^{\tau^n/n!} \\ &= e^{-\omega\tau/2} \sum_{n \text{ even / odd}} \frac{1}{n!} \left(\tau K e^{-S_{\rm inst}/\hbar}\right)^n . \end{aligned} \tag{3.40}$$

Finally, performing the summation, one obtains the transition amplitude

$$G(a,\pm a;\tau) \simeq C e^{-\omega\tau/2} \begin{cases} \cosh\left(\tau K e^{-S_{\rm inst.}/\hbar}\right) \\ \sinh\left(\tau K e^{-S_{\rm inst.}/\hbar}\right) \end{cases} \tag{3.41}$$

where C is some factor that depends in a non–exponential way on the transition time.

Before we turn to a discussion of the physical content of this result, let us check the self–consistency of our central working hypothesis — the diluteness of the instanton gas. To this end, consider the representation of G in terms of the partial amplitudes (3.40). To determine the typical number of instantons contributing to the sum, one may make use of the fact that, for a general sum $\sum_n c_n$ of positive quantities $c_n > 0$, the 'typical' value of the summation index can be estimated as $\langle n\rangle \equiv \sum_n c_n n / \sum_n c_n$. With the abbreviation $X \equiv \tau K e^{-S_{\rm inst}/\hbar}$, the application of this estimate to our current sum yields

$$\langle n\rangle \equiv \frac{\sum_n n X^n/n!}{\sum_n X^n/n!} = X,$$

where we have used the fact that, as long as $\langle n\rangle \gg 1$, the even/odd distinction in the sum is irrelevant. Thus, we can infer that the average instanton density, $\langle n\rangle/\tau = K e^{-S_{\rm inst}/\hbar}$ is both exponentially small in the instanton action $S_{\rm inst}$, and independent of τ confirming the validity of our diluteness assumptions above.

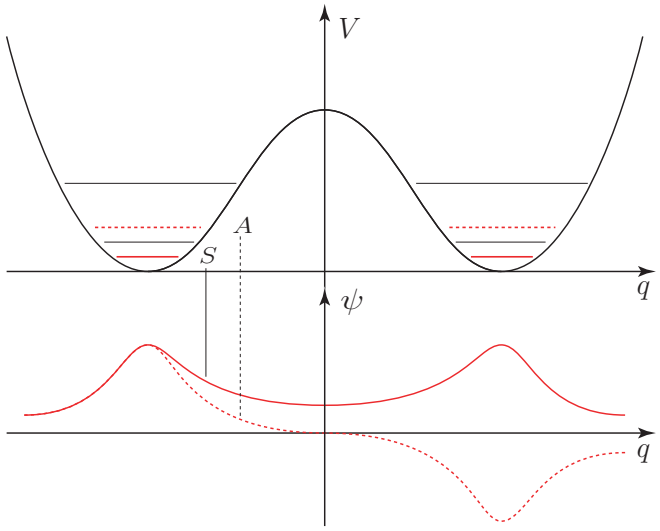


Figure 3.9: Quantum states in the double well: Dashed: Harmonic oscillator states. Solid: Exact eigenstates.

Finally, let us discuss how the form of the transition amplitude (3.41) can be understood in physical terms. To this end, let us reconsider the basic structure of the problem we are dealing with (see Fig. 3.9). While there is no coupling across the barrier, the Hamiltonian has two independent, oscillator–like sets of low lying eigenstates sitting in the two local minima. Allowing for a weak inter–barrier coupling, the oscillator ground states (like all higher states) split into a doublet of a symmetric and an antisymmetric eigenstate, $|S\rangle$ and $|A\rangle$ with energies ϵ_A and ϵ_S, respectively. Focusing on the low energy sector formed by the ground state doublet, we can express the transition amplitudes (3.32) as

$$G(a,\pm a;\tau) \simeq \langle a|\Big(|S\rangle e^{-\epsilon_S \tau/\hbar}\langle S| + |A\rangle e^{-\epsilon_A \tau/\hbar}\langle A|\Big)|\pm a\rangle.$$

Setting $\epsilon_{A/S} = \hbar\omega/2 \pm \Delta\epsilon/2$, where $\Delta\epsilon$ represents the tunnel-splitting, the symmetry properties $|\langle a|S\rangle|^2 = |\langle -a|S\rangle|^2 = C/2$ and $\langle a|A\rangle\langle A|-a\rangle = -|\langle a|A\rangle|^2 = -C/2$ imply that

$$G(a,\pm a;\tau) \simeq \frac{C}{2}\left(e^{-(\hbar\omega-\Delta\epsilon)\tau/2\hbar} \pm e^{-(\hbar\omega+\Delta\epsilon)\tau/2\hbar}\right) = Ce^{-\omega\tau/2}\begin{cases}\cosh(\Delta\epsilon\tau/\hbar)\\ \sinh(\Delta\epsilon\tau/\hbar)\end{cases}.$$

Comparing this expression with Eq. (3.41) the interpretation of the instanton calculation becomes clear: At long times, the transition amplitude engages the two lowest states — the symmetric and anti–symmetric combination of the two oscillator ground states. The energy splitting $\Delta\epsilon$ accommodates the energy shift due to the tunneling between the two wells. Remarkably, the effect of tunneling was obtained from a purely classical picture (formulated in imaginary time!). The instanton calculation also produced a prediction for the tunnel splitting of the energies, viz.

$$\Delta\epsilon = \hbar K \exp(-S_{\rm inst}/\hbar),$$

which, up to the prefactor, agrees with the result of a WKB–type analysis of the tunnel process.

Before leaving this section, two general remarks on instantons are in order:

- ▷ In hindsight, was the approximation scheme used above consistent? In particular, terms at second order in $\hbar$ were neglected, while terms non–perturbative in $\hbar$ (the instanton) were kept. Yet, the former typically give rise to a larger correction to the energy than the latter. However, the large perturbative shift effects the energies of the symmetric and antisymmetric state equally. The instanton contribution gives the *leading* correction to the splitting of the levels. It is the latter which is likely to be of more physical significance.

- ▷ Secondly, it may — legitimately — appear as though the development of the machinery above was a bit of an "overkill" for describing a simple tunnelling process. As a matter of fact, the basic result (3.41) could have been obtained in a simpler way by more elementary means (using, for example, the WKB method). Why then did we discuss instantons at such length? One reason is that, even within a purely quantum mechanical framework, the instanton formulation of tunnelling is much stronger than WKB. The latter represents, by and large, an uncontrolled approximation. In general it is hard to tell whether WKB results are accurate or not. In contrast, the instanton approximation to the path integral is controlled by a number of well–defined expansion parameters. For example, by going beyond the semiclassical approximation and/or softening the diluteness assumption, the calculation of the transition amplitudes can, in principle, be driven to arbitrary accuracy.

- ▷ A second, and for our purposes, more important motivation is that instanton techniques are of crucial importance within higher dimensional field theories (here we regard the path integral formulation of quantum mechanics as a 0 space +1 time = 1–dimensional field theory). The reason is that instantons are intrinsically non–perturbative objects, which is to say that instanton solutions to stationary phase equations describe a type of physics that cannot be obtained by a perturbative expansion around a non–instanton sector of the theory. (For example, the bouncing

orbits in the example above cannot be incorporated into the analysis by doing a kind of perturbative expansion around a trivial orbit.) This non–perturbative nature of instantons can be understood by topological reasoning:

Relatedly, one of the features of the instanton analysis above was that the *number* of instantons involved was a stable quantity; 'stable' in the sense that by including perturbative fluctuations around the n instanton sector, say, one does not connect with the $n+2$ sector. Although no rigorous proof of this statement has been given, it should be heuristically clear: a trajectory involving n bounces between the hills of the inverted potential cannot be smoothly connected with one of a different number. Suppose for instance we would forcably attempt to interpolate between two paths with different bounce numbers: Inevitably, some of the intermediate configurations would be charged with actions that are far apart from any stationary phase like value. Thus, the different instanton sectors are separated by an energetic barrier that cannot be penetrated by smooth interpolation and, in this sense, they are **topologically distinct**.

▷ INFO. **Fluctuation determinant**: Our analysis above provided a method to extract the tunneling rate between the quantum wells to a level of exponential accuracy. However, in some applications, it is useful to compute the exponential prefactor K. Although such a computation follows the general principles outlined above and implemented explicitly for the single well, there are some idiosyncracies in the tunneling system which warrant discussion.

According to the general principles outlined in section 3.2.2, integrating over Gaussian fluctuations around the saddle–point field configurations, the contribution to the transition amplitude from the n–instanton section is given by

$$G_n = J\mathrm{det}\left(-m\partial_\tau^2 + V''(q_{\mathrm{cl},n})\right)\, e^{-nS_{\mathrm{inst.}}/\hbar}$$

where $q_{\mathrm{cl},n}(\tau)$ represents an n–instanton configuration and J the normalisation. Now, in the zero instanton sector, the evaluation of the functional determinant recovers the familiar harmonic oscillator result, $G(0,0;\tau) = (m\omega/\pi\hbar)^{1/2}\exp[-\omega\tau/2]$. Let us now consider the one instanton sector of the theory. To evaluate the functional determinant, one must consider the spectrum of the operator $-m\partial_\tau^2 + V''(q_{\mathrm{cl},1})$. Differentiating the defining equation for $q_{\mathrm{cl},1}$ (3.34), one may confirm that

$$\left(-m\partial_\tau^2 + V''(q_{\mathrm{cl},1})\right)\partial_\tau q_{\mathrm{cl},1} = 0,$$

i.e. the function $\partial_\tau q_{\mathrm{cl},1}$ presents a zero mode of the operator!. Physically, the origin of the zero mode is elucidated by noting that a translation of the instanton along the time axis, $q_{\mathrm{cl},1}(\tau) \to q_{\mathrm{cl},1}(\tau+\delta\tau)$ should leave the action approximately invariant. However, for small $\delta\tau$, $q_{\mathrm{cl},1}(\tau+\delta\tau) \simeq q_{\mathrm{cl},1}(\tau) + \delta\tau\partial_\tau q_{\mathrm{cl},1}$, i.e. to first order, the addition of the increment function $\partial_\tau q_{\mathrm{cl},1}$ leaves the action invariant, and $\delta\tau$ is a 'zero mode coordinate'.

With this interpretation, it becomes clear how to repair the formula for the fluctuation determinant. While the Gaussian integral over fluctuations is controlled for the non–zero eigenvalues, its execution for the zero mode must be rethought. Indeed, by integrating over the coodinate of the instanton, viz. $\int_0^\tau d\tau_0 = \tau$, one finds that the contribution to the transition amplitude in the one instanton sector is given by

$$J\tau\sqrt{\frac{S_{\mathrm{inst.}}}{2\pi\hbar}}\mathrm{det}'\left[-m\partial_\tau^2 + V''(q_{\mathrm{cl},1})\right]^{-1/2} e^{-S_{\mathrm{inst.}}/\hbar}$$

where the prime indicates the exclusion of the zero mode from the determinant, and the factor $\sqrt{S_{\rm inst.}/2\pi\hbar}$ reflects the Jacobian associated with the change to a new set of integration variables which contains the zero mode coordinate τ as one of its elements.[20] To fix the, as yet, undetermined coupling constant J, we normalize by the fluctuation determinant of the (imaginary time) harmonic oscillator, i.e. we use the fact that (cf. section 3.3.1), for the harmonic oscillator, the return amplitude evaluates to $G(0,0,\tau) = J\,\det(m(-\partial_\tau^2+\omega^2)/2)^{-1/2} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\omega\tau/2}$, where the first/second representation is the imaginary time variant of Eq. (3.30)/Eq.(3.31). Using this result, and noting that the zero mode analysis above generalizes to the n–instanton sector, we find that the pre–exponential constant K used in our analysis of the double well problem above affords the explicit representation

$$K = \omega\sqrt{\frac{S_{\rm inst.}}{2\pi\hbar}}\left[\frac{m\omega^2 \det'\left[-m\partial_\tau^2 + V''(q_{\rm cl,1})\right]}{\det\left[-m\partial_\tau^2 + m\omega^2\right]}\right]^{-1/2}.$$

Naturally, the instanton determinant depends sensitively on the particular nature of the potential $V(q)$. For the quartic potential $V(q) = m\omega^2(x^2-a^2)^2/8a^2$, it may be confirmed that the

$$\frac{m\omega^2 \det'\left[-m\partial_\tau^2 + V''(q_{\rm cl,1})\right]}{\det\left[-m\partial_\tau^2 + m\omega^2\right]} = \frac{1}{12},$$

while $S_{\rm inst} = \sqrt{2/3}\,m\omega a^2$. For further details of the calculation, we refer to, e.g., Zinn-Justin.

Escape From a Metastable Minimum: "Bounces"

The instanton gas approximation for the double well system can be easily adapted to explore the problem of quantum mechanical tunneling from a metastable state such as that presented by an unstable nucleus. In particular, suppose one wishes to estimate the "survival probability" of a particle captured in a metastable minimum of a one–dimensional potential such as that shown in Fig. 3.10.

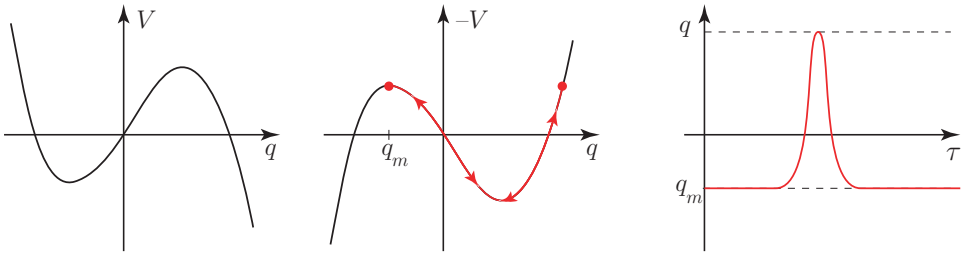


Figure 3.10: Effective potential showing a metastable minimum together with the inverted potential and a sketch of a bounce solution. To obtain the tunnelling rate it is necessary to sum over a dilute gas of bounce trajectories.

According to the path integral scheme, the survival probability, defined by the probability amplitude to remain at the potential minimum q_m, i.e. the propagator $G(q_m, q_m; t)$,

[20] For an explicit calculation of this Jacobian see, e.g., J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Oxford University Press, 1993).

can be evaluated by making use of the Euclidean time formulation of the Feynman path integral. As with the double well, in the Euclidean time formalism, the dominant contribution to the transition probability arises from the classical path minimising the action corresponding to the inverted potential (see Fig. 3.10). However, in contrast to the double well potential, the classical solution takes the form of a '**bounce**' (i.e. the particle spends only a short time away from the potential minimum — there is only one metastable minimum of the potential). As with the double well, one can expect mutliple bounce trajectories to present a significant contribution. Summing over all bounce trajectories (note that in this case we have an exponential series — no even/odd parity effect), one obtains the survival probability

$$G(q_m, q_m; \tau) = Ce^{-\omega\tau/2} \exp\left[\tau K e^{-S_{\rm bounce}/\hbar}\right].$$

Applying an analytic continuation to real time, one finds $G(\theta_m, \theta_m; t) = Ce^{-i\omega t/2} \exp[-\frac{\Gamma}{2}t]$, where the decay rate is given by $\Gamma/2 = |K|e^{-S_{\rm bounce}/\hbar}$. (Note that on physical grounds we can see that K must be imaginary.[21]

▷ Exercise. Consider a heavy nucleus having a finite rate of α-decay. The nuclear forces can be considered very short-ranged so that the rate of α particle emission is controlled by tunneling under a Coulomb barrier. Taking the effective potential to be spherically symmetric with a deep minimum core of radius r_0 beyond which it decays as $U(r) = 2(Z-1)e^2/r$ where Z is the nuclear charge, find the temperature of the nuclei above which α-decay will be thermally assisted if the energy of the emitted particles is E_0. Estimate the mean energy of the α particles as a function of temperature.

▷ Exercise. A uniform electric field E is applied perpendicular to the surface of a metal with work function W. Assuming that the electrons in the metal describe a Fermi gas of density n, with exponential accuracy, find the tunneling current at zero temperature ("cold emission"). Show that, effectively, only electrons with energy near the Fermi level are tunneling. With the same accuracy, find the current at finite temperature ("hot emission"). What is the most probable energy of tunneling electrons as function of temperature?

3.3.3 †Tunneling of Quantum Fields: 'Fate of the False Vacuum'

▷ Additional Example: Hitherto we have focussed on applications of the Feynman path integral to the quantum mechanics of isolated point–like particles. In this setting, the merit of the path integral scheme over, say, standard perturbative methods or the 'WKB' approach is perhaps not compelling. Therefore, by way of motivation, let us here present an example which builds upon the structures elucidated above and which illustrates the power of the path integral method.

[21] In fact, a more careful analysis shows that this estimate of the decay rate is too large by a factor of 2 (for further details see, e.g., Coleman, *Aspects of Symmetry: Selected Erice Lectures*, CUP.)

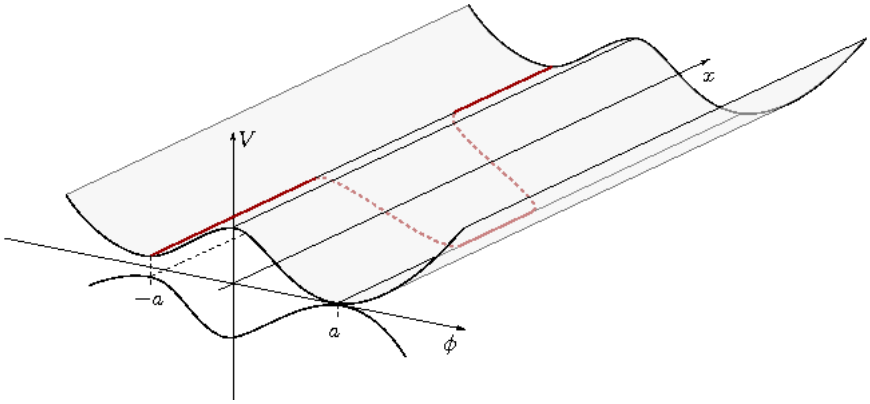


Figure 3.11: Snapshot of a field configuration $\phi(x, t = \text{const.})$ in a potential landscape with two nearly degenerate minima. For further discussion, see the text.

To this end, let us consider a theory involving a continuous classical field which can adopt two homogeneous equilibrium states with different energy densities: To be concrete, one may consider an harmonic chain confined to one or other minimum of an asymmetric quasi one–dimensional 'gutter–like' double well potential (see Fig. 3.11). When quantised, the state of higher energy density becomes unstable through barrier penetration — it is said to be a "false vacuum".[22] Specifically, drawing on our discussion of the harmonic chain in chapter 1, let us consider a quantum system specified by the Hamiltonian density

$$\hat{\mathcal{H}} = \frac{\hat{\pi}^2}{2m} + \frac{k_s a^2}{2}(\partial_x \hat{\phi})^2 + V(\hat{\phi}), \tag{3.42}$$

where $[\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar\delta(x - x')$. Here we have included a potential $V(\phi)$ which, in the present case, assumes the form of a double well. The inclusion of a weak bias $-f\phi$ into $V(\phi)$ identifies a stable and a metastable potential minimum. Previously, we have seen that, in the absence of the confining potential, the quantum string exhibits low–energy collective wave–like excitations — phonons. In the confining potential, these harmonic fluctuations are rendered massive. However, drawing on the quantum mechanical principles established in the single–particle system, one might assume that the string tunnels freely between the two potential minima. To explore the capacity of the system to tunnel, let us suppose that, at some time $t = 0$, the system adopts a field configuration in which the string is located in the (metastable) minimum of the potential at, say, $\phi = -a$. What is the probability that the *entire* string of length L will tunnel across the barrier into the potential minimum at $\phi = a$ in a time t?

▷ INFO. The tunneling of fields between nearly degenerate ground state plays a role in numerous physical contexts. By way of example, consider a **superheated liquid**. In this context, the 'false' vacuum is the liquid state, and the true one the gaseous phase. The role of the field is taken by the local density distribution in the liquid. Thermodynamic fluctuations trigger the continuous appearance of vapor bubbles in the liquid. For bubbles of too small a

[22] For a detailed discussion of the history and ramifications of this idea, we refer on the original insightful paper by Sidney Coleman, *Fate of the false vacuum: semiclassical theory*, Phys. Rev. D **15**, 2929 (1977). Indeed, many of the ideas developed in this work were anticipated in an earlier analysis of metastability in the context of classical field theories by J. S. Langer, *Theory of the condensation point*, Ann. Phys. (N.Y.) **41**, 108 (1967).

diameter, the gain in volume energy is outweighed by the surface energy cost — the bubble will collapse. However, for bubbles beyond a certain critical size, the energy balance is positive. The bubble will grow and, eventually, swallow the entire mass density of the system; the liquid has vaporised or, more formally, the density field has tunneled[23] from the false ground state into the true one.

More speculative (but also potentially more damaging) manifestations of the phenomenon have been suggested in the context of **cosmology**:[22] What if the big bang released our universe not into its true vacuum configuration but into a state separated by a huge barrier from a more favourable sector of the energy landscape. In this case, everything would depend on the tunneling rate: *'If this time scale is of the order of milliseconds, the universe is still hot when the false vacuum decays... if this time is on the order of years, the decay will lead to a sort of secondary big bang with interesting cosmological consequences. If this time is of the order of 10^9 years, we have occasion for anxiety.'* (S. Coleman, *ibid.*).

Previously, for the point–particle system, we have seen that the transition probability between the minima of the double well is most easily accessed by exploring the classical field configurations of the Euclidean time action. In the present case, anticipating to some extent our discussion of the quantum field integral in the next chapter, the Euclidean time action associated with the Hamiltonian density (3.42) assumes the form[24]

$$S[\phi] = \int_0^T d\tau \int_0^L dx \left[\frac{m}{2}(\partial_\tau \phi)^2 + \frac{k_s a^2}{2}(\partial_x \phi)^2 + V(\phi) \right] ,$$

where the time integral runs over the interval $[0, T = it]$. Here, for simplicity, let us assume that the string obeys periodic boundary conditions in space, viz. $\phi(x + L, \tau) \equiv \phi(x, \tau)$. To estimate the tunneling amplitude, we will explore the survival probability of the metastable state imposing the boundary conditions $\phi(x, \tau = 0) = \phi(x, \tau = T) = -a$ on the path integral. Once again, when the potential barrier is high, and the time T is long, one may assume that the path integral is dominated by the saddle–point field configuration of the Euclidean action. In this case, varying the action with respect to the field $\phi(x, \tau)$, one obtains the classical equation of motion

$$m\partial_\tau^2 \phi + k_s a^2 \partial_x^2 \phi = \partial_\phi V(\phi) ,$$

which must be solved subject to the boundary conditions above.

Now, motivated by our consideration of the point–particle problem, one might seek a solution in which the string tunnels as a single rigid entity without 'flexing'. However, it is evident from the spatial translational invariance of the system that the instanton action would scale with the system size L. In the infinite system $L \to \infty$, such a trajectory would therefore not contribute significantly to the tunneling amplitude. Instead, one must consider a different type of field configurataion in which the transfer of the chain is by degree: Elements of the string cross the

[23] At this point, readers should no longer be confused regarding the mentioning of 'tunneling' in the context of a classical system: Within the framework of the path integral, the classical partition sum maps onto the path integral of a fictitious quantum system. It is the tunneling of the latter we have in mind.

[24] Those readers who wish to develop a more rigorous formulation of the path integral for the string may either turn to the discussion of the field integral in the next chapter or, alternatively, may satisfy themselves of the validity of the Euclidean action by (re–)discretisating the harmonic chain, presenting the transition amplitude as a series of Feynman path integrals for each element of the string and, finally, taking the continuum limit.

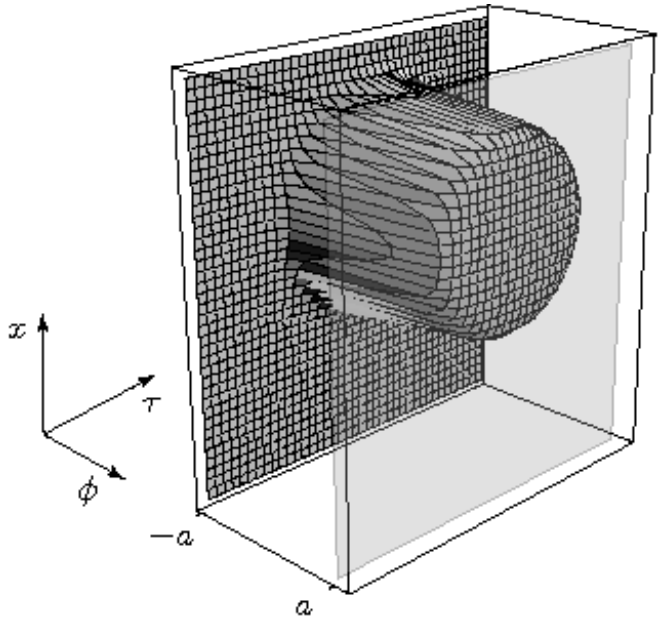


Figure 3.12: On the tunneling between two nearly degenerate vacuum states. As time moves on, a one–dimensional 'world sheet' sweeps through a circular structure in Euclidean space time. This results in the inflation of a 'bubble' of the true vacuum state in real space.

barrier in a consecutive sequence as two outwardly propagating 'domain walls' (see the figure where the emergence of such a double–kink configuration is shown as a function of space and time; notice the spherical shape of the resulting space–time droplet — a consequence of the rotational symmetry of the rescaled problem). Such a field configuration can be motivated from symmetry considerations by noting that, after rescaling $x \mapsto v_s x$ (where $v_s = \sqrt{k_s a^2/m}$ denotes the classical sound wave velocity), the saddle–point equation assumes the isotropic form $m\partial^2\phi = \partial_\phi V(\phi)$, where $\partial^2 = \partial_\tau^2 + \partial_x^2$. Then, setting $r = \sqrt{x^2 + (\tau - T/2)^2}$, and sending $(T, L) \to \infty$, the space–time rotational symmetry suggests a solution of the form $\phi = \phi(r)$ where $\phi(r)$ obeys the radial diffusion equation

$$\partial_r^2\phi + \frac{1}{r}\partial_r\phi = \partial_\phi V\,,$$

with the boundary condition $\lim_{r\to\infty}\phi(r) = -a$. This equation describes the one–dimensional motion of a particle in a potential $-V$ and subject to a strange "friction force" $-r^{-1}\partial_r\phi$ whose strength is inversely proportional to 'time' r.

To understand the profile of the non–trivial bounce solution of the problem, suppose that at time $r = 0$ the particle has been released at rest at a position slightly to the left of the (inverted) potential maximum at a. After rolling through the potential minimum it will climb the potential hill at $-a$. Now, the initial position may be fine tuned such that the viscous damping of the particle compensates for the excess potential energy (which would otherwise make the particle overshoot and disappear to infinity): there exists a solution where the particle starts close to $\phi = a$ and eventually winds up at $\phi = -a$, in accord with the imposed boundary conditions. In general, the analytical solution for the bounce depends sensitively on the form of the confining potential. However, while we assume that the well asymmetry imposed by external potential $-f\phi$ is small, the radial equation may be considerably simplified. In this limit, one may invoke a

"thin-wall" approximation in which one assumes that the bounce configuration is described by a domain wall of thickness Δr, at a radius $r_0 \gg \Delta r$ separating an inner region where $\phi(r < r_0) = a$ from the outer region where $\phi(r > r_0) = -a$. In this case, and to lowest order in an expansion in f, the action of the friction force is immaterial, i.e. we may set $m\partial_r^2\phi = \partial_\phi V$ — the very instanton equation formulated earlier for the point–particle system!

Then, when substituted back into S, one finds that the bounce (or kink–like) solution is characterised by the Euclidean action

$$S = v_s \left[2\pi r_0 S_{\text{inst.}} - \pi r_0^2\, 2af\right]$$

where $S_{\text{inst.}}$ denotes the action of the instanton associated with the point–particle system (3.36), and the last term accommodates the effect of the potential bias on the field configuration. Crucially, one may note that the instanton contribution to the action scales with the circumference of the domain wall in the space–time, while that of the potential bias scales with the area of the domain. From this scaling dependence, it is evident that, however small is the external force f, at large enough r_0, the contribution of the second term will always outweigh the first and the string will tunnel from the metastable minimum to the global minimum of the potential. More precisely, the optimal size of domain is found by minimising the action with respect to r_0. In doing so, one finds that $r_0 = S_{\text{inst.}}/2af$. Then, when substituted back into the action, one obtains the tunneling rate

$$\Gamma \sim \exp\left[-\frac{1}{\hbar}\frac{\pi v_s S_{\text{inst.}}^2}{2af}\right].$$

From this result, one can conclude that, in the absence of an external force f, the tunneling of the string across the barrier is *completely quenched*! In the zero temperature unbiased system, the symmetry of the quantum Hamiltonian is broken: The ground state exhibits a two–fold degeneracy in which the string is confined to one potential minimum or another.

The ramifications of the tunneling amplitude suppression can be traced to the statistical mechanics of the corresponding classical system: As emphasized in section 3.2.1, any Euclidean time path integral of a d–dimensional system can be identified with the statistical mechanics of a classical system $(d+1)$–dimensional problem. In the double well system, the Euclidean time action of the point–particle quantum system is isomorphic to the one–dimensional realisation of the classical Ising ferromagnet, viz.

$$\beta H_{\text{Ising}} = \int_0^L d^d\mathbf{x}\left[\frac{t}{2}m^2 + um^4 + \frac{K}{2}(\nabla m)^2\right] \tag{3.43}$$

Translated into this context, the saddle–point (or mean–field) analysis suggests that the system will exhibit a spontaneous symmetry breaking to an ordered phase ($m \neq 0$) when the parameter t (the reduced temperature) becomes negative. However, drawing on our analysis of the quantum point–particle system, in the thermodynamic limit, we see that fluctuations (non–perturbative in temperature) associated with instanton field configurations of the Hamiltonian $m(x)$ may restore the symmetry of the system and destroy long–range order at any finite temperature $1/\beta$. Whether this happens or not depends on the competition between the energy cost of instanton creation and the entropy gained by integrating over the instanton zero mode coordinates. It turns out that in $d = 1$, the latter wins, i.e. the system is 'disordered' at any finite temperature. In contrast, for $d \geq 2$, the creation of instantons is too costly, i.e. the system will remain in its energetically preferred ground state.

3.3.4 †Tunneling in a Dissipative Environment

▷ Additional Example: In the condensed matter context it is, of course, infeasible to completely divorce a system from its environment. Indeed, in addition to the dephasing effect of thermal fluctuations, the realization of quantum mechanical phenomena depends sensitively on the strength and nature of the coupling to the external degrees of freedom. For example, the tunneling of an atom from one interstitial site in a crystal to another is likely to be heavily influenced by its coupling to the phonon degrees of freedom that characterise the crystal lattice. By exchanging energy with the phonons, which act in the system as an external bath, a quantum particle can loose its phase coherence and with it, its quantum mechanical character. Beginning with the seminal work of Caldeira and Leggett,[25] there have been numerous theoretical investigations of the effect of an enviroment on the quantum mechanical properties of a system. Such effects are particularly acute in systems where the quantum mechanical degree of freedom is *macroscopic* such as the magnetic flux trapped in a superconducting quantum interference device (SQUID). In the following, we will show that the Feynman path integral provides a natural (and almost unique) setting in which the effects of the environment on a microscopic or macroscopic quantum mechanical degree of freedom can be explored.

Before we begin, let us note that the phenomenon of macroscopic quantum tunneling represents an extensive and still active area of research recently reinvigorated by the burgeoning field of quantum computation. By contrast, our discussion here will be necessarily limited in scope, targeting a particular illustrative application, and highlighting only the guiding principles. For a more thorough and detailed discussion, we refer the reader to one of the many comprehensive reviews.[26]

Caldeira–Leggett Model

Previously, we have discussed the ability of the Feynman path integral to describe quantum mechanical tunneling of a particle q across a potential barrier $V(q)$. In the following, we will invoke the path integral to explore the capacity for quantum mechanical tunneling when the particle is coupled to degrees of freedom of an external environment. Following Calderia and Leggett's original formulation, let us represent the environment by a bath of N quantum harmonic oscillators characterised by a set of frequencies $\{\omega_\alpha\}$,

$$\hat{H}_{\rm bath}[q_\alpha] = \sum_\alpha^N \left[\frac{\hat{p}_\alpha^2}{2m_\alpha} + \frac{m_\alpha}{2}\omega_\alpha^2 q_\alpha^2 \right] .$$

For simplicity, let us suppose that in the leading approximation, the coupling of the particle to the degrees of freedom of the bath is linear such that $\hat{H}_{\rm c}[q, q_\alpha] = -\sum_\alpha^N f_\alpha[q] q_\alpha$, where $f_\alpha[q]$ represents some function of the particle coordinate q. Expressed as a Feynman path integral, the survival probability of a particle confined to a metastable minimum at a position $q = a$, and coupled to an external environment, can then be expressed as ($\hbar = 1$)

$$\langle a|e^{-i\hat{H}t/\hbar}|a\rangle = \int_{q(0)=q(t)=a} Dq\; e^{iS_{\rm part.}[q]} \int Dq_\alpha\; e^{iS_{\rm bath}[q_\alpha]+iS_{\rm c}[q,q_\alpha]} ,$$

[25] A. O. Calderia and A. J. Leggett, *Influence of Dissipation on Quantum Tunneling in Macroscopic Systems*, Phys. Rev. Lett. **46**, 211 (1981).

[26] See, e.g., A. J. Leggett *et al.*, *Dynamics of the dissipative two–state system*, Rev. Mod. Phys **48**, 357 (1976), and the text by Weiss [**?**].

where $\hat{H} = \hat{H}_{\rm part.} + \hat{H}_{\rm bath} + \hat{H}_{\rm c}$ denotes the total Hamiltonian of the system,

$$S_{\rm part.}[q] = \int_0^t dt \left[\frac{m}{2}\dot{q}^2 - V(q)\right], \qquad S_{\rm bath}[q_\alpha] = \int_0^t dt \sum_\alpha \frac{m_\alpha}{2}\left[\dot{q}_\alpha^2 - \omega_\alpha^2 q_\alpha^2\right],$$

denote, respectively, the action of the particle and bath, while

$$S_{\rm coupling}[q, q_\alpha] = -\int_0^t dt \sum_\alpha f_\alpha[q] q_\alpha - \int dt \sum_a \frac{f_\alpha[q]^2}{2 m_a \omega_a^2},$$

represents their coupling.[27] Here we assume that the functional integral over $q_\alpha(t)$ is taken over all field configurations of the bath while, as before, the path integral on $q(t)$ is subject to the boundary conditions $q(0) = q(t) = a$.

To reveal the effect of the bath on the capacity for tunneling of the particle, it is instructive to integrate out fluctuations q_α and thereby obtain an effective action for q. Fortunately, being Gaussian in the coordinates q_α, the integration can performed straightforwardly. Although not crucial, since we are dealing with quantum mechanical tunneling, it is useful to transfer to the Euclidean time representation. Taking the boundary conditions on the fields $q_\alpha(\tau)$ to be periodic on the interval $[0, T^{-1} \equiv \beta]$, it may be confirmed that the Gaussian functional integral over q_α induces a time non–local interaction of the particle (exercise) $\langle a|e^{-i\hat{H}t/\hbar}|a\rangle = \int Dq\, e^{-S_{\rm eff}[q]}$ where a constant of integration has been absorbed into the measure and

$$S_{\rm eff}[q] = S_{\rm part.}[q] + \frac{1}{2T}\sum_{\omega_n,\alpha} \frac{\omega_n^2 f_\alpha[q(\omega_n)] f_\alpha[q(-\omega_n)]}{m_\alpha \omega_\alpha^2(\omega_\alpha^2 + \omega_n^2)}.$$

Here, the sum $\sum_{\omega_n}$ runs over the discrete set of Fourier frequencies $\omega_n = 2\pi n/\beta$ with n integer.[28] By integrating out the bath degrees of freedom, the particle action acquires an induced contribution. To explore its effect on dissipation and tunneling, it is necessary to specialise our discussion to a particular form of coupling.

In the particular case that the coupling to the bath is linear, viz. $f_\alpha[q(\tau)] = c_\alpha q(\tau)$, the effective action assumes the form (exercise)

$$\boxed{S_{\rm eff}[q] = S_{\rm part.}[q] - T\int_0^\beta d\tau\, d\tau'\, K(\tau - \tau') q(\tau) q(\tau')}$$

where $K(\tau) = \int_0^\infty \frac{d\omega}{\pi} J(\omega) D_\omega(\tau)$, $J(\omega) = \frac{\pi}{2}\sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha}\delta(\omega - \omega_\alpha)$, and

$$D_\omega(\tau) = -\sum_{\omega_n} \frac{2\omega_n^2}{\omega(\omega^2 + \omega_n^2)} e^{i\omega_n \tau},$$

resembles the Green function of a boson with energy $\hbar\omega$. Physically, the non–locality of the action is easily understood: By exchanging fluctuations with the external bath, a particle can

[27] The second term in the coupling action has been added to keep the effect of the environment minimally invasive (purely dissipative). If it would not be present, the coupling to the oscillator degrees of freedom would effectively *shift* the extremum of the particle potential, i.e. change its potential landscape. Exercise: substitute the solutions of the Euler–Lagrange equations $\delta_{q_\alpha} S[q, q_\alpha] = 0$ — computed for a fixed realization of q — into the action to obtain the said shift.

[28] More preceisely, anticipating our discussion of the Matsubara frequency representation, we have defined the Fourier decomposition on the Euclidean time interval T, viz. $q(\tau) = \sum_m q_m e^{i\omega_m \tau}$, $q_m = T\int_0^\beta d\tau q(\tau) e^{-i\omega_m \tau}$, where $\omega_m = 2\pi m/\beta$ with m integer.

affect a self–interaction, retarded in time. Taken as a whole, the particle and the bath maintain quantum phase coherence. However, when projected onto the particle degree of freedom, the total energy of the system appears to fluctuate and the phase coherence of the particle transport is diminished. To explore the properties of the dissipative action, it is helpful to separate the non–local interaction according to the identity $q(\tau)q(\tau') = [q^2(\tau) + q^2(\tau')]/2 - [q(\tau) - q(\tau')]^2/2$. The former squared contribution presents an innocuous renormalisation of the potential $V(q)$ and, applying equally to the classically allowed motion as well as quantum tunneling, presents an unobservable perturbation. Therefore, we will suppose that its effect has been absorbed into a redefinition of the particle potential $V(q)$. By contrast, the remaining contribution is always positive.

The particular form of the "spectral function" $J(\omega)$ may be obtained either from an *a priori* knowledge of the microscopic interactions of the bath, or phenomenologically, it can be inferred from the structure of the classical damped equations of motion. For example, for a system subject to an "ohmic" dissipation (where, in real time, the classical equations of motion obtain a dissipative term $-\eta\dot{q}$ with a "friction coefficient" η), one has $J(\omega) = \eta|\omega|$ for all frequencies smaller than some characteristic cut–off (at the scale of the inverse Drude relaxation time of the environment). By contrast, for a defect in a three–dimensional crystal, interaction with acoustic phonons present a frequency dependence of ω^3 or ω^5 depending on whether ω is below or above the Debye frequency.

▷ Info. Consider, for example, the coupling of a particle to a continuum of bosonic modes whose spectral density $J(\omega) = \frac{\eta}{8}\omega$ grows linearly with frequency. In this case,

$$K(\omega_n) = -\frac{\eta\omega_n^2}{8\pi}\int_0^\infty d\omega \frac{1}{\omega^2+\omega_n^2} = -\frac{\eta}{4}|\omega_n|.$$

describes **Ohmic dissipation** of the particle. Fourier transforming this expression we obtain

$$K(\tau) = -\frac{\pi T\eta}{4}\frac{1}{\sin^2(\pi T\tau)} \overset{\tau\ll T^{-1}}{\simeq} -\frac{\eta}{4\pi T}\frac{1}{\tau^2}, \tag{3.44}$$

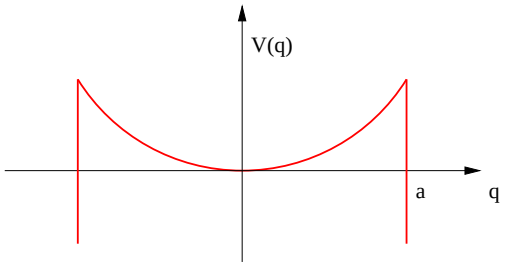
i.e. a strongly time non–local 'self–interaction' of the particle.

Disssipative Quantum Tunneling

Returning to the particular problem at hand, previously, we have seen that the tunneling rate of a particle from a metastable potential minimum can be inferred from the extremal field configurations of the Euclidean action: the bounce trajectory. To explore the effect of the dissipative coupling, it is necessary to understand how it revises the structure of the bounce solution. Now, in general, the non–local character of the interaction inhibits access to an exact solution of the classical equation of motion. In such cases, the effect of the dissipative coupling can be explored perturbatively or with the assistance of the renormalisation group (see the discussion in section **??**). However, by tailoring our choice potential $V(\phi)$, we can gain some intuition about the more general situation.

To this end, let us consider a particle of mass m confined in a metastable minimum by a (semi–infinite) *harmonic* potential trap (see figure),

$$V(q) = \begin{cases} m\omega_c^2 q^2/2 & 0 < q \le a\,, \\ -\infty & q > a\,. \end{cases}$$



Further, let us assume that the environment imparts an ohmic dissipation with a damping or viscosity η. To keep our discussion general, let us consider the combined impact of dissipation and temperature on the rate of tunneling from the potential trap. To do so, following Langer[29] it is natural to investigate the "quasi–equilibrium" quantum partition function $\mathcal{Z}$ of the combined system. In this case, the tunneling rate appears as an imaginary contribution to the free energy $F = -T \ln \mathcal{Z}$, viz. $\Gamma = -2\mathrm{Im}\, F$.

Drawing on the path integral, the quantum partition function of the system can be presented as a functional integral $\mathcal{Z} = \int_{q(\beta)=q(0)} Dq e^{-S_{\rm eff}}$ where, as we have seen above, for ohmic coupling, the Euclidean action assumes the form

$$S_{\rm eff}[q] = \int_0^\beta d\tau \, \left(\frac{m}{2}\dot{q}^2 + V(q) \right) + \frac{\eta}{4\pi} \int_0^\beta d\tau \, d\tau' \, \left(\frac{q(\tau) - q(\tau')}{\tau - \tau'} \right)^2 .$$

Once again, to estimate the tunneling rate, we will suppose that the barrier is high and the temperature is low so that the path integral is dominated by stationary configurations of the action. In this case, one may identify three distinct solutions: In the first place, the particle may remain at $q = 0$ poised precariously on the maximum of the inverted harmonic potential. Contributions from this solution and the associated harmonic fluctuations reproduce terms in the quantum partition function associated with states of the *closed* harmonic potential trap. Secondly, there exists a singular solution in which the particle remains at the minimum of the inverted potential, i.e. perched on the potential barrier. The latter presents a negligible contribution to the quantum partition function and can be neglected. Finally, there exists a bounce solution in which the particle injected at a position q inside the well accelerates down the inverted potential gradient, is reflected from the potential barrier, and returns to the initial position q in a time β. While, in the limit $\beta \to \infty$, the path integral singles out the boundary condition $q(0) = q(\beta) \to 0$, at finite β, the boundary condition will depart from 0 in a manner that depends non–trivially on the temperature. It is this general bounce solution which governs the decay rate.

Since, in the inverted potential, the classical bounce trajectory stays within the interval over which the potential is quadratic, a variation of the Euclidean action with respect to $q(\tau)$ obtains the classical equation of motion

$$-m\ddot{q} + m\omega_c^2 q + \frac{\eta}{\pi} \int_0^\beta d\tau' \, \frac{q(\tau) - q(\tau')}{(\tau - \tau')^2} = A\delta(\tau - \beta/2) \, ,$$

where the term on the right hand side of the equation imparts an impulse which changes discontinuously the velocity of the particle, while the coefficient A is chosen to ensure symmetry of the bounce solution on the Euclidean time interval. Turning to the Fourier representation, the solution of the saddle–point equation then assumes the form

$$q_n = ATe^{-i\omega_n \beta/2} g(\omega_n), \qquad g(\omega_n) \equiv [m(\omega_n^2 + \omega_c^2) + \eta|\omega_m|]^{-1}. \tag{3.45}$$

[29] J. S. Langer, `Ben:...`

Imposing the condition that $q(\tau = \beta/2) = a$, one finds that $A = a/f$ where $f \equiv T\sum_n g(\omega_n)$. Finally, the action of the bounce is given by

$$S_{\rm bounce} = \frac{1}{2T}\sum_n (m(\omega_n^2 + \omega_c^2) + \eta|\omega_m|)|q_n|^2 = \frac{a^2}{2f}. \tag{3.46}$$

(a) To make sense of these expressions, as a point of reference, let us first determine the **zero temperature tunneling rate in the absence of dissipation**, viz. $\eta \to 0$ and $\beta \to \infty$. In this case, the (Matsubara) frequency summation translates to the continuous integral, $f = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, g(\omega) = (2m\omega_c)^{-1}$. Using this result, the bounce action (3.46) takes the form $S_{\rm bounce} = m\omega_c a^2$. As one would expect, the tunnelling rate $\Gamma \sim e^{-S_{\rm bounce}}$ is controlled by the ratio of the potential barrier height $m\omega_c^2 a^2/2$ to the attempt frequency ω_c. Also notice that the bounce trajectory is given by

$$q(\tau) = \frac{a}{f}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\; e^{i\omega(\tau-\beta/2)} g(\omega) = a\, e^{-\omega_c|\tau-\beta/2|}\,,$$

i.e. as expected from our discussion in section 3.3.2, the particle spends only a time $1/\omega_c$ in the under barrier region.

(b) Now, restricting attention to the zero temperature limit, let us consider the **influence of dissipation** on the nature of the bounce solution and the capacity for tunneling. Focussing on the limit in which the dynamics of the particle is overdamped, $\eta \gg m\omega_c$, $f = \int_{-\infty}^{\infty} g(\omega) \simeq \frac{2}{\pi\eta}\ln(\eta/m\omega_c)$, which implies $S_{\rm bounce} = \frac{\pi\eta a^2}{4\ln[\eta/(m\omega_c)]}$. In particular, this result shows that, in the limit $\eta \to \infty$, the coupling of the particle to the ohmic bath leads to an *exponential* suppression of the tunneling rate while only a weak dependence on the jump frequency persists. Physically, this result is easy to rationalise: Under–barrier tunneling is a feature of the quantum mechanical system. By transferring energy to and from the external bath, the phase coherence of the particle is lost. At zero temperature, the tunneling rate becomes suppressed and the particle confined.

(c) Let us now consider the **influence of temperature on the tunneling rate when the dissipative coupling is inactive** $\eta \to 0$. In this case, the discrete frequency summation takes the form[30] $f = T\sum_n g(\omega_n) = \frac{\coth(\beta\omega_c/2)}{2\omega_c m}$. Using this result, one obtains the action $S_{\rm bounce} = m\omega_c a^2 \tanh(\beta\omega_c/2)$. In the low temperature limit $\beta \to \infty$, $S_{\rm bounce} = m\omega_c a^2$ as discussed above. At high temperatures $\beta \to 0$, as expected, one recovers a classical activated dependence of the escape rate, viz. $S \simeq \beta m\omega_c^2 a^2/2$.

(d) Finally, let us briefly remark on the **interplay of thermal activation with ohmic dissipation**. Applying the the Euler-Maclaurin formula $\sum_{m=0}^{\infty} f(m) = \int_0^{\infty} dx\, f(x) + \frac{f(0)}{2} - \frac{f'(0)}{12} + \ldots$ to relate discrete sums over Matsubara frequencies to their zero temperature integral limits, one finds that $S_{\rm bounce}(T) - S_{\rm bounce}(T=0) \propto \eta T^2$. This shows that, in the dissipative regime, an increase in temperature diminishes the tunneling rate with a scale proportion to the damping.

This concludes our cursory discussion of the application of the Feynman path integral to dissipative quantum tunneling. As mentioned above, our brief survey was able only to touch upon the broad field of research. Those interested in learning more about the field of macroscopic

[30] For details on how to implement the discrete frequency summation, see the info block on p 137 below.

quantum tunneling are referred to the wider literature. To close this chapter, we turn now to our penultimate application of the path integral — quantum mechanical spin.

3.3.5 †Path Integral for Spin

▷ Additional Example: The quantum mechanics of a spin 1/2–particle is a standard example in introductory courses. Indeed, there is hardly any other system whose quantum mechanics is as easy to formulate. Given that, it is perhaps surprising that for a long time the spin problem defied all attempts to cast it in path integral form: Feynman, the architect of the path integral, did not succeed in incorporating spin into the new formalism. It took several decades to fill this gap (for a review of the early history up to 1980, see Schulman's text [20]), and a fully satisfactory formulation of the subject was obtained no earlier than 1988. (The present exposition follows closely the lines of the review by Michael Stone, *Supersymmetry and the Quantum Mechanics of Spin*, Nucl. Phys. **B 314**, 557 (1989).)

Why then is it so difficult to find a path integral of spin? In hindsight it turns out that the spin path integral is in fact no more complex than any other path integral, it merely appears to be a bit unfamiliar. The reason is that, on the one hand, the integrand of the path integral is essentially the exponentiated *classical* action whilst, on the other, the **classical mechanics of spin** is a subject that is not standard in introductory or even advanced courses. In other words, the path integral approach must, by necessity, lead to an unusual object. The fact that the *classical* mechanics of spin is hardly ever mentioned is not only related to the common view that spin is something 'fundamentally quantum' but also to the fact that the mechanics of a classical spin (see below) cannot be expressed within the standard formulation of Hamiltonian mechanics, i.e. there is no formulation in terms of a set of globally defined coordinates and equally many global momenta. It is therefore inevitable that one must resort to the (less widely applied) symplectic formulation of Hamiltonian mechanics.[31] However, as we will see below, the classical mechanics of spin can nevertheless be quite easily understood physically.

Besides attempting to elucidate the connections beween quantum and classical mechanics of spin, there is yet an other motivation for discussing the spin path integral. Pretending that we have forgotten essential quantum mechanics, we will formulate the path integral ignoring the fact that spin quantum numbers are half integer or integer. The quantization of spin will then be derived in hindsight, by way of a *geometric consideration*. In other words, the path integral formulation demonstrates how quantum mechanical results can be obtained by geometric rather than standard algebraic reasoning. Finally, the path integral of spin will serve as a basic platform on which our analysis of higher dimensional spin systems below will be based.

A reminder of finite–dimensional SU(2)–representation theory

In order to formulate the spin path integral, it is neccessary to recapitulate some facts regarding the role of SU(2) in quantum mechanics. The special unitary group in two dimensions, SU(2), is defined as $SU(2) = \{g \in \mathrm{Mat}(2\times 2, \mathbb{C}) | g^\dagger g = \mathbf{1}_2, \det g = 1\}$, where $\mathbf{1}_2$ is the two–dimensional unit matrix. Counting independent components one finds that the group has three free real

[31] Within this formulation, the phase space is regarded as a differential manifold with a symplectic structure (cf. Arnold's text on classical mechanics [**?**]). (In the case of spin, this manifold is the two—sphere S^2.)

parameters or, equivalently, that its Lie algebra, su(2), is three dimensional. As we have seen, the basis vectors of the algebra — the group generators — $\hat{S}^i$, $i = x, y, z$ satisfy the closure relation $[\hat{S}^i, \hat{S}^j] = i\epsilon_{ijk}\hat{S}^k$, where ϵ_{ijk} is the familiar fully antisymmetric tensor. An alternative, and often more useful basis representation of su(2) is given by the spin **raising and lowering operators**, $\hat{S}^{\pm} = (\hat{S}^x \pm i\hat{S}^y)/2$. Again, as we have seen earlier, the algebra $\{\hat{S}^+, \hat{S}^-, \hat{S}^z\}$ is defined by the commutation relations $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$, $[\hat{S}^z, \hat{S}^{\pm}] = \pm 2\hat{S}^{\pm}$.

Each group element can be uniquely parametrized in terms of the exponentiated algebra. For example, in the **Euler angle representation**,[32] the group is represented as

$$\mathrm{SU}(2) = \left\{ g(\phi,\theta,\psi) = e^{-i\phi\hat{S}_3}e^{-i\theta\hat{S}_2}e^{-i\psi\hat{S}_3} \,\middle|\, \phi,\psi \in [0,2\pi], \theta \in [0,\pi] \right\}.$$

The Hilbert space $\mathcal{H}_S$ of a quantum spin represents an irreducible representation space of SU(2). Within the spaces $\mathcal{H}_S$, SU(2) acts in terms of representation matrices (which will be denoted by g) and the matrix representations of its generators $\hat{S}_i$. The index S is the so–called weight of the representation (physically: the total spin).[33] Within each $\mathcal{H}_S$, there is a distinguished state, a state of highest weight $|\uparrow\rangle$, which is defined as the (normalized) eigenstate of $\hat{S}^z$ with maximum eigenvalue, S (physically: a spin state polarised in the 3–direction, often denoted as $|S, S_z = S\rangle$, where m is the azimuthal quantum number). Owing to the irreducibility of the representation, each (normalized) state of the Hilbert space $\mathcal{H}_S$ can be obtained by applying the Euler–angle–parameterized elements of the representation to the maximum weight state.

Being a compact group, SU(2) can be integrated over; i.e. it makes sense to define objects like $\int_{\mathrm{SU}(2)} dg f(g)$, where f is some function of g and dg is a realization of a group measure.[34] Among the variety of measures that can be defined in principle, the (unique) **Haar measure** plays a distinguished role. It has the convenient property that it is invariant under left and right multiplication of g by fixed group elements; i.e.

$$\forall h \in \mathrm{SU}(2): \qquad \int dg f(gh) = \int dg f(hg) = \int dg f(g),$$

where, for notational simplicity, we have omitted the subscript in $\int_{\mathrm{SU}(2)}$.

Construction of the path integral

With this background, we are now in a position to formulate the Feynman path integral for quantum mechanical spin. To be specific, let us consider a particle of spin S subject to the Hamiltonian

$$\hat{H} = \mathbf{B} \cdot \hat{\mathbf{S}},$$

[32]

Leonhard Euler 1707–1783: Swiss mathematician and physicist, one of the founders of pure mathematics. He not only made decisive and formative contributions to the subjects of geometry, calculus, mechanics, and number theory but also developed methods for solving problems in observational astronomy and demonstrated useful applications of mathematics in technology and public affairs.

[33] The index S is defined in terms of the eigenvalues of the Casimir operator (physically: the total angular momentum operator) $\hat{\mathbf{S}}^2 \equiv \sum_i \hat{\mathbf{S}}_i^2$ according to the relation $\forall |s\rangle \in \mathcal{H}_S: \ \hat{\mathbf{S}}^2|s\rangle = S(S+1)|s\rangle$.

[34] To define group measures in a mathematically clean way, one makes use of the fact that (as a Lie group) SU(2) is a 3–dimensional differentiable manifold. Group measures can then be defined in terms of the associated volume form (see the primer in differential geometry on page **??** below).

where $\mathbf{B}$ is a magnetic field and $\hat{\mathbf{S}} \equiv (\hat{S}_1, \hat{S}_2, \hat{S}_3)$ is a vector of spin operators in the spin–S representation. Our aim is to calculate the imaginary time path integral representation of the quantum partition function $\mathcal{Z} \equiv \mathrm{tr}\, e^{-\beta \hat{H}}$. In constructing the path integral we will follow the general strategy outlined at the end of section 3.2.3, i.e. the first step is to represent $\mathcal{Z}$ as $\mathcal{Z} = \mathrm{tr}\,(e^{-\epsilon \hat{H}})^N$, where $\epsilon = \beta/N$. Next, we have — the most important step in the construction — to insert a suitably chosen resolution of identity between each of the factors $e^{-\epsilon \hat{H}}$. A representation that will lead us directly to the final form of the path integral is specified by

$$\mathrm{id.} = C \int dg\, |g\rangle\langle g| \tag{3.47}$$

where 'id.' represents the unit operator in $\mathcal{H}_S$, $\int dg$ is a group integral over the Haar measure, C is some constant and $|g\rangle \equiv g|\uparrow\rangle$ is the state obtained by letting the representation matrix g act on the maximum weight state $|\uparrow\rangle$ (cf. the summary of the SU(2) representation theory above).

Of course it remains to be verified that the integral (3.47) is indeed proportional to the unit operator. That this is so follows from **Schur's lemma** which states that if, and only if, an operator $\hat{A}$ commutes with all representation matrices of an irreducible group representation (in our case the gs acting in the Hilbert space $\mathcal{H}_S$), $\hat{A}$ is either zero or proportional to the unit matrix. That the group above integral fulfils the global commutativity criterion follows from the properties of the Haar measure: $\forall h \in \mathrm{SU}(2)$,

$$h \int dg|g\rangle\langle g| = \int dg|hg\rangle\langle g| \overset{\text{Haar}}{=} \int dg|hh^{-1}g\rangle\langle h^{-1}g| = \int dg|g\rangle\langle g|h.$$

Thus, $\int dg|g\rangle\langle g|$ is, indeed, proportional to the unit operator. The proportionality constant appearing in (3.47) will not be of any concern to us — apart from the fact that it is non–zero.[35]

Substituting the resolution of identity into the time–sliced partition function and making use of the fact that

$$\begin{aligned}\langle g_{i+1}|e^{-\epsilon \mathbf{B}\cdot\hat{\mathbf{S}}}|g_i\rangle &\simeq \langle g_{i+1}|g_i\rangle - \epsilon\langle g_{i+1}|\mathbf{B}\cdot\hat{\mathbf{S}}|g_i\rangle \overset{\langle g_i|g_i\rangle = 1}{=} 1 - \langle g_i|g_i\rangle + \langle g_{i+1}|g_i\rangle - \epsilon\langle g_{i+1}|\mathbf{B}\cdot\hat{\mathbf{S}}|g_i\rangle \\ &\simeq \exp\Big(\langle g_{i+1}|g_i\rangle - \langle g_i|g_i\rangle - \epsilon\langle g_{i+1}|\mathbf{B}\cdot\hat{\mathbf{S}}|g_i\rangle\Big),\end{aligned}$$

one obtains

$$\mathcal{Z} = \lim_{N\to\infty} \int_{g_N = g_0} \prod_{i=0}^{N} dg_i \exp\left[-\epsilon \sum_{i=0}^{N-1}\left(-\frac{\langle g_{i+1}|g_i\rangle - \langle g_i|g_i\rangle}{\epsilon} + \langle g_{i+1}|\mathbf{B}\cdot\hat{\mathbf{S}}|g_i\rangle\right)\right].$$

Taking the limit $N \to \infty$, the latter can be cast in path integral form,

$$\boxed{\mathcal{Z} = \int Dg \exp\left[-\int_0^\beta d\tau \left(-\langle \partial_\tau g|g\rangle + \langle g|\mathbf{B}\cdot\hat{\mathbf{S}}|g\rangle\right)\right]} \tag{3.48}$$

where the $\mathcal{H}_S$–valued function $|g(\tau)\rangle$ is the continuum limit of $|g_i\rangle$. Eq. (3.48) is our final, albeit somewhat over–compact, representation of the path integral. In order to give this expression some physical interpretation, we need to examine more thoroughly the meaning of the states $|g\rangle$.

[35] Actually, the constant C can be straightforwardly computed by taking the trace of (3.47) which leads to $C =$(dimension of the representation space)/(volume of the group).

In the literature, the states $|g\rangle$ expressed in the Euler–angle representation

$$\boxed{|\widetilde{g}(\phi,\theta,\psi)\rangle \equiv e^{-i\phi\hat{S}_3}e^{-i\theta\hat{S}_2}e^{-i\psi\hat{S}_3}|\uparrow\rangle}$$

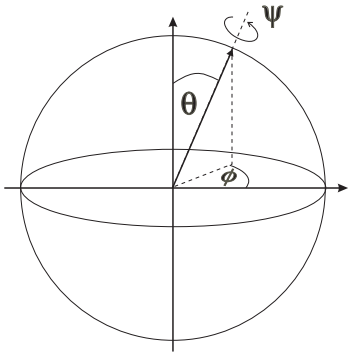
are referred to as **spin coherent states**. Before discussing the origin of this terminology, it is useful to explore the algebraic structure of these states. First, note that the maximum weight state $|\uparrow\rangle$ is, by definition, an eigenstate of $\hat{S}_3$ with maximum eigenvalue S. Thus, $|\widetilde{g}(\phi,\theta,\psi)\rangle \equiv e^{-i\phi\hat{S}_3}e^{-i\theta\hat{S}_2}|\uparrow\rangle e^{-i\psi S}$ and the angle ψ enters the coherent state merely as a phase or gauge factor. By contrast, the two remaining angles θ and ϕ act through true rotations. Now, the angular variables $\phi \in [0, 2\pi[$ and $\theta \in [0, \pi[$ define a standard representation of the two–sphere. In view of the fact that (up to normalization factors) the states $|g(\phi,\theta,\psi)\rangle$ cover the entire Hilbert space $\mathcal{H}_S$, we are led to suspect that the latter bears structural similarity with a sphere.[36] To substantiate this view, let us compute the expectation values

$$n_i \equiv \langle\tilde{g}(\phi,\theta,\psi)|\hat{S}_i|\tilde{g}(\phi,\theta,\psi)\rangle, \qquad i = 1, 2, 3. \tag{3.49}$$

To this end, we first derive an auxiliary identity which will spare us much of the trouble that will arise in expanding the exponentials appearing in the definition of $|\widetilde{g}\rangle$. Making use of the general identity ($i \neq j$)

$$e^{-i\phi\hat{S}_i}\hat{S}_j e^{i\phi\hat{S}_i} = e^{-i\phi[\hat{S}_i,\ ]}\hat{S}_j = \hat{S}_j\cos\phi + \epsilon_{ijk}\hat{S}_k\sin\phi, \tag{3.50}$$

where the last equality follows from the fact that $\cos x\,(\sin x)$ contain x in even (odd) orders and $[\hat{S}_j,\ ]^2\hat{S}_i = \hat{S}_i$, it is a straightforward matter to obtain (exercise) $\mathbf{n} = S(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, i.e. $\mathbf{n}$ is the product of S and a unit vector parameterized in terms of spherical coordinates. This is the key to understanding the terminology 'spin coherent states': The states $|\widetilde{g}(\phi,\theta,\psi)\rangle$ represent the closest approximation of a classical angular momentum one can form out of spin operators (see the figure).



Let us now see what happens if we employ the Euler angle representation in formulating the path integral. A first and important observation is that the path integral is gauge invariant — in the sense that it does not depend on the U(1)–phase, ψ. As for the $\mathbf{B}$–dependent part of the action, the gauge invariance is manifest: Eq. (3.49) implies that

$$S_B[\phi,\theta] \equiv \int_0^\beta d\tau\langle\tilde{g}|\mathbf{B}\cdot\hat{\mathbf{S}}|\tilde{g}\rangle = \int_0^\beta d\tau\langle g|\mathbf{B}\cdot\hat{\mathbf{S}}|g\rangle = S\int_0^\beta d\tau\,\mathbf{n}\cdot\mathbf{B} = SB\int_0^\beta d\tau\cos\theta.$$

[36] There is a group theoretical identity behind this observation, viz. the isomorphism $\mathrm{SU}(2) \simeq S^2\times\mathrm{U}(1)$, where U(1) is the 'gauge' subgroup contained in SU(2).

Here, we have introduced the gauge–independent part $|g\rangle$ of the state vector by setting $|\widetilde{g}\rangle \equiv |g\rangle \exp(-iS\psi)$ or,equivalently, $|g(\phi,\theta)\rangle \equiv e^{-i\phi\hat{S}_3}e^{-i\theta\hat{S}_2}|\uparrow\rangle$. Substituting this representation into the first term of the action of (3.48), one obtains

$$\begin{aligned} S_{\rm top}[\phi,\theta] &\equiv -\int_0^\beta d\tau\langle\partial_\tau\tilde{g}|\tilde{g}\rangle = -\int_0^\beta d\tau\langle\partial_\tau e^{-iS\psi}g|ge^{-iS\psi}\rangle \\ &= -\int_0^\beta d\tau\left(\langle\partial_\tau g|g\rangle - iS\,\partial_\tau\psi\langle g|g\rangle\right) = -\int_0^\beta d\tau\langle\partial_\tau g|g\rangle, \end{aligned} \tag{3.51}$$

where the last equality holds because $\langle g|g\rangle = 1$ is constant and ψ is periodic in β. As an important intermediate result we have found that the path integral is overall gauge invariant or, equivalently, that the path integral is one over paths living on the two–sphere (rather than the entire group manifold SU(2)). This finding is reasuring in the sense that a degree of freedom living on a sphere comes close to what one might intuitively expect to be the classical counterpart of a quantum particle with conserved angular momentum.

Let us now proceed by exploring the action of the path integral. Using the auxiliary identity (3.50) it is a straightforward matter to show that

$$S_{\rm top}[\phi,\theta] = -\int_0^\beta d\tau\langle\partial_\tau g|g\rangle = -iS\int_0^\beta d\tau\,\partial_\tau\phi\cos\theta = iS\int_0^\beta d\tau\,\partial_\tau\phi(1-\cos\theta). \tag{3.52}$$

Combining this with the **B**–dependent term discussed above, one obtains

$$\boxed{S[\theta,\phi] = S_B[\phi,\theta] + S_{\rm top}[\phi,\theta] = S\int_0^\beta d\tau\,[B\cos\theta + i(1-\cos\theta)\partial_\tau\phi]} \tag{3.53}$$

for the action of the path integral for spin.

▷ Exercise. Derive the Euler–Lagrange equations asasociated with this action. Show that they are equivalent to the **Bloch equations** $i\partial_\tau\mathbf{n} = \mathbf{B}\times\mathbf{n}$ of a spin with expectation value $\langle\mathbf{S}\rangle = S\mathbf{n}$ subject to a magnetic field. Here, $\mathbf{n}(\phi,\theta)\in S^2$ is the unit vector defined by the two angles ϕ,θ.

Analysis of the action

To formulate the second term in the action (3.53) in a more suggestive way, we note that the velocity of the point $\mathbf{n}$ moving on the unit sphere is given by $\dot{\mathbf{n}} = \dot{\theta}\hat{\mathbf{e}}_\theta + \dot{\phi}\sin\theta\,\hat{\mathbf{e}}_\phi$, where $(\hat{\mathbf{e}}_r,\hat{\mathbf{e}}_\theta,\hat{\mathbf{e}}_\phi)$ form a spherical orthonormal system. We can thus rewrite Eq. (3.52) as

$$S_{\rm top}[\phi,\theta] = iS\int_0^\beta d\tau\,\dot{\mathbf{n}}\cdot\mathbf{A} = iS\oint_\gamma d\mathbf{n}\cdot\mathbf{A}, \tag{3.54}$$

where

$$\mathbf{A} = \frac{1-\cos\theta}{\sin\theta}\hat{\mathbf{e}}_\phi. \tag{3.55}$$

Notice that, in spite of its compact appearance, Eq. (3.54) does not represent a coordinate invariant formulation of the action $S_{\rm top}$. (The field $\mathbf{A}(\phi,\theta)$ explcitly depends on the coordinates (ϕ,θ).) In fact, the action $S_{\rm top}$ *cannot* be expressed in a coordinate invariant manner, for reasons deeply rooted in the topology of the two–sphere.

A second observation is that (3.54) can be read as the (Euclidean time) action of a particle of charge S moving under the influence of a vector potential $\mathbf{A}$ (cf., for example, Ref. [**?**].) Using standard formulae of vector calculus (cf. Ref. [**?**]) one finds $\mathbf{B}_{\rm m} \equiv \nabla \times \mathbf{A} = S\mathbf{e}_r$, i.e. our particle moves in a radial magnetic field of constant strength S. Put differently, the particle moves in the field of a magnetic 'charge' of strength 4π centered on the origin of the sphere.

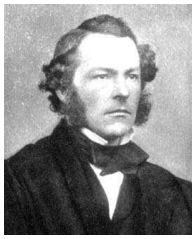
▷ INFO. If you find this statement difficult to reconcile with the Maxwell equation $\nabla \cdot \mathbf{B} = 0 \leftrightarrow \int_S \mathbf{B} \cdot dS$ for any closed surface S, notice that $\nabla \cdot \mathbf{B} = \nabla \cdot (\nabla \times \mathbf{A}) = 0$ holds only if $\mathbf{A}$ is non–singular. However, the vector potential (3.55) is manifestly singular along the line $(r, \theta = \pi)$ through the south pole of the sphere. The physical picture behind this singularity is as follows: Imagine an infinitely thin solenoid running from $r = \infty$ through the south pole of the sphere to its center. Assuming that the solenoid contains a magnetic flux 4π, the center of the sphere becomes a source of magnetic flux, the so–called **Dirac monopole**. This picture is consistent with the presence of a field $\mathbf{B} = \mathbf{e}_r$. It also explains the singularity of $\mathbf{A}$ along the string. (Of course, the solenoidal construction does not lead to the prediction of a genuine monopole potential: Somewhere, at $r = \infty$, our auxiliary magnetic coil has to end, and this is where the flux lines emanating from the point $r = 0$ terminate.) The postulate of a flux line at the singularity of $\mathbf{A}$ merely helps to reconcile the presence of a radial magnetic field with the principles of electrodynamics. However, as far as our present discussion goes, this extra structure is not essential, i.e. we may simply interpret $r = 0$ as the position of a magnetic 'charge'.

To explore the consequences of this phenomenon, we apply Stokes' theorem[37]

$$S_{\rm top}[\mathbf{n}] = iS \oint_\gamma \mathbf{n} \cdot \mathbf{A} = iS \oint_{A_{\gamma,n}} dS \cdot (\nabla \times \mathbf{A}) = iS \oint_{A_{\gamma,n}} dS \cdot \mathbf{e}_r = iSA_{\gamma,n}. \tag{3.56}$$

Here, $A_{\gamma,n}$ is the domain on the two–sphere which (a) has the curve γ as its boundary, and (b) contains the north pole (see the figure). The integral produces the area of this surface which we again denote by $A_{\gamma,n}$. Curiously, the action $S_{\rm top}$ is but a measure of the area bounded by the curve $\gamma : \tau \mapsto \mathbf{n}(\tau)$. However, simple as it is, this result should raise some suspicion: By assigning a designated role to the *northern* hemisphere of the sphere some symmetry breaking, not present in the original problem, has been introduced. Indeed, we might have defined our action by $S_{\rm top}[\phi, \theta] = iS \oint_\gamma d\mathbf{n} \cdot \mathbf{A}'$ where $\mathbf{A}' = -\frac{1+\cos\theta}{\sin\theta}\hat{e}_\phi = \mathbf{A} - 2\nabla\phi$ differs from $\mathbf{A}$ only by a gauge transformation.[38] The newly defined vector potential is non–singular in the *southern* hemisphere, so that application of Stokes' theorem leads to the conclusion $S_{\rm top}[\mathbf{n}] = -iS \int_{A_{\gamma,s}} dS \cdot \mathbf{B}_m =$

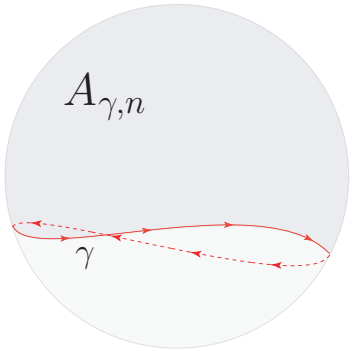
[37]



George Gabriel Stokes 1819–1903: As Lucasian Professor of Mathematics at Cambridge Stokes established the science of hydrodynamics with his law of viscosity (1851), describing the velocity of a small sphere through a viscous fluid. Furthermore, he investigated the wave theory of light, named and explained the phenomenon of fluorescence, and theorised an explanation of the Fraunhofer lines in the solar spectrum.

[38] You may, with some justification, feel uneasy about the fact that ϕ is not a true 'function' on the sphere (or, alternatively, about the fact that $\int d\mathbf{n} \cdot \nabla\phi = \phi(\beta) - \phi(0)$ may be a non–vanishing multiple of 2π). We will return to the discussion of this ambiguity shortly. (Notice that a similarly hazardous manipulation is performed in the last equality of Eq. (3.52).)

$-iSA_{\gamma,s}$. Here, $A_{\gamma,s}$ is the area of a surface bounded by γ but covering the *south* pole of the sphere. The absolute minus sign is due to the outward orientation of the surface $A_{\gamma,s}$.



One has to concede that the result obtained for the action S_{top} depends on the chosen gauge of the monopole vector potential! The difference between the northern and the southern variant of our analysis is given by

$$iS\int_{A_{\gamma,n}} dS\cdot\mathbf{B}_m + iS\int_{A_{\gamma,s}} dS\cdot\mathbf{B}_m = iS\int_{S^2} dS\cdot\mathbf{e}_r = 4\pi iS,$$

where we have made use of the fact that $A_{\gamma,n}\cup A_{\gamma,s} = S^2$ is the full sphere. At first sight, it looks as if our analysis has led us to a gauge dependent, and therefore pathological result. Let's recall, however, that physical quantities are determined by the *exponentiated* action $\exp(iS[\mathbf{n}])$ and not by the action itself. Now, S is either integer or half integer which implies the factor $\exp(4\pi iS) = 1$ is irrelevant. In the operator representation of the theory, spin quantization follows from the representation theory of the algebra su(2). It is a 'non–local' feature, in the sense that the action of the spin operators on all eigenstates has to be considered to fix the dimensionality $2S+1$ of $\mathcal{H}_S$. In hindsight, it is thus not too surprising that the same information is encapsulated in a 'global' condition (gauge invariance) imposed on the action of the path integral.

Summarizing, we have found that the classical dynamics of a spin is that of a massless point particle on a sphere coupled to a monopole field $\mathbf{B}_m$. We have seen that the vector potential of the latter cannot be globally continuous on the full sphere. More generally, the phase space S^2 cannot be represented in terms of a global system of 'coordinates and momenta' which places it outside the scope of traditional treatments of classical mechanics. This probably explains the failure of early attempts to describe the spin in terms of a path integral or, equivalently, in terms of a Hamiltonian action.

In chapter **??** we will use the path action (3.53) as a building block for our construction of the field theory of higher dimensional spin systems. However, before concluding this section, let us make some more remarks on the curious properties of the monopole action S_{top}: Contrary to all other Euclidean actions encountered thus far, the action (3.54) is imaginary. In fact, it will stay imaginary upon Wick rotation $\tau \to it$ back to real times. More generally, S_{top} is invariant under the rescaling $\tau \to c\tau$, and invariant even under arbitrary reparameterizations $\tau \to g(\tau) \equiv \tau'$. This invariance is a hallmark of a **topological term**. Loosely speaking (see chapter **??** for a deeper discussion), a topological term is a contribution to the action of a field theory that depends on the global geometry of a field configuration rather than on its local structure. In contrast, 'conventional' operators in field theoretical actions measure the energy cost of dynamical or spatial field fluctuations. In doing to they must relate to a specific spatio–temporal reference frame, i.e. they cannot be invariant under reparamaterisation.

Summarizing our results, we have found that:

1. The classical action of a spin is one of a massless particle (there is no standard kinetic energy term in (3.48)) moving on a unit sphere. The particle carries a magnetic moment of magnitude S. It is coupled to (a) a conventional magnetic field via its magnetic moment, and (b) to a monopole field via its orbital motion. Note that we have come, finally, to a position which hints at the difficulties plaguing attempts to formulate a classical mechanics of spin. The vector potential of a monopole, $\mathbf{A}$, cannot be globally defined on the entire sphere. The underlying physical reason is that, by the very nature of the monopole (flux going radially outwards everywhere), the associated vector potential must be singular at one point of the surface.[39] As a consequence, the classical phase space of the system, the sphere, cannot be covered by a global choice of coordinate system. (Unlike most standard problems of classical mechanics there is no system of globally defined 'p's and 'q's.) This fact largely spoils a description within the standard — coordinate oriented — formulation of Hamiltonian mechanics (cf. the discussion in the article by Stone).

2. Terms akin to the monopole contribution to the spin action appear quite frequently within path integral formulations of systems with non–trivial topology (like the two–sphere above). Depending on the particular context under consideration, one distinguishes between **Wess–Zumino–Witten (WZW) terms,**[40] **θ–terms, Chern–Simons terms** and a few other terms of topological origin. What makes these contributions generally important is that the value taken by these terms depends *only* on the topology of a field configuration but not on structural details.

As a final application of the path integral, we turn now to the consideration of problems in which the dynamics of the classical system is, itself, non–trivial.

3.3.6 †Trace Formulae and Quantum Chaos

▷ Additional Example: Introductory courses on classical mechanics usually convey the impression that dynamical systems behave in a regular and, at least in principle, mathematically predictable way. However, experience shows that the majority of dynamical processes in nature do not conform with this picture: Partly, or even fully chaotic motion (i.e. motion that

[39] To better understand this point, consider the integral of $\mathbf{A}$ along an infinitesimal closed curve γ on the sphere. *If* $\mathbf{A}$ were globally continuous, we would have two choices to transform the integral into a surface integral over $\mathbf{B}$; an integral over the 'large' or the 'small' surface area bounded by γ. The monopole nature of $\mathbf{B}$ would demand that both integrals are proportional to the respective area of the integration domain which, by assumption, are different $\rightsquigarrow$ contradiction. The resolution of this paradox is that $\mathbf{A}$ must be discontinuous at one point on the sphere, i.e. we cannot globally set $\mathbf{B} = \nabla \times \mathbf{A}$ and the choice of the integration area is prescribed by the condition that it must not encompass the singular point.

[40]

Edward Witten 1951–: 1990 Fields Medal for his work in superstring theory. He made significant contributions to Morse theory, supersymmetry, and knot theory. Additionally, he explored the relationship between quantum field theory and the differential topology of manifolds of two and three dimensions.

depends in a singular and, thereby, in an essentially unpredictable way on initial conditions) is the rule rather than the exception. In view of the drastic differences in the observable behaviour of classically integrable and chaotic systems, an obvious question arises: In what way does the *quantum* phenomenology of chaotic systems differ from that associated with integrable dynamics? This question defines the field of **quantum chaos**.

Understanding signatures of classically chaotic motion in quantum mechanics is an issue not only of conceptual, but also of great practical relevance impinging on areas such as quantum electron transport in condensed matter systems: The inevitable presence of impurities and imperfections in any macroscopic solid renders the long–time dynamics of electronic charge carriers chaotic. Relying on a loose interpretation of the Heisenberg principle, $\Delta t \sim \hbar/\Delta E$, i.e. the relation between *long*–time dynamical behaviour and *small* scale structures in energy, one would expect that signatures of chaotic quantum dynamics are especially important in the low–energy response in which one is usually interested. This expectation has been confirmed for innumerable observables related to low temperature electronic transport in solid state systems.

Disordered conducting media represent but one example of a wide class of dynamical systems with long–time chaotic dynamics. Indeed, recent experimental advances have made it possible to realize a plethora of effectively *non–disordered* chaotic dynamical systems in condensed matter devices. For example, employing modern semiconductor device technology, it has become possible to manufacture small two–dimensional conducting systems, of a size $\mathcal{O}(< 1\mu\,\mathrm{m})$ and of almost any geometric shape. Here, the number of imperfections can be reduced to a negligible minimum, i.e. electrons propagate ballistically along straight trajectories, as in a billiard. The smallness of the devices further implies that the ratio between Fermi wavelength and system size is of $\mathcal{O}(10^{-1} - 10^{-3})$, i.e. while semiclassical concepts will surely be applicable, the wave aspects of quantum propagation remain visible. In recent years, the experimental and theoretical study of electron transport in such **quantum billiards** has emerged as a field in its own right.

How then *can* signatures of chaotic dynamics in quantum systems be sought? The most fundamental characteristic of a quantum system is its spectrum. Although not a direct observable, it determines the majority of properties accessible to measurement. On the other hand, it is clear that the manifestations of chaos we are looking for must relate back to the classical dynamical properties of the system. The question then is, *how can a link between classical mechanics and quantum spectra be drawn?* This problem is tailor made for analysis by path integral techniques.

Semiclassical Approximation to the Density of States

The close connection between the path integral and classical mechanics should be evident from the previous sections. However, to address the problem raised above, we still need to understand how the path integral can be employed to analyse the spectrum of a quantum system. The latter are described by the (single–particle) **density of states**

$$\rho(\epsilon) = \mathrm{tr}\,\delta(\epsilon - \hat{H}) = \sum_a \delta(\epsilon - \epsilon_a)\,, \tag{3.57}$$

where $\{\epsilon_a\}$ represents the complete set of energy levels. To compute the sum, one commonly employs a trick based on the **Dirac identity**,

$$\lim_{\delta \searrow 0} \frac{1}{x + i\delta} = -i\pi\delta(x) + \mathcal{P}\frac{1}{x}\,, \tag{3.58}$$

where $\mathcal{P}(1/x)$ denotes for the principal part of $1/x$. Taking the imaginary part of (3.58), Eq. (3.57) can be represented as $\rho(\epsilon) = -\frac{1}{\pi}\,\mathrm{Im}\,\sum_a \frac{1}{\epsilon^+ - \epsilon_a} = -\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{tr}\,(\frac{1}{\epsilon^+ - \hat{H}})$, where $\epsilon^+ \equiv \epsilon + i\delta$

and the limit $\lim_{\delta\searrow 0}$ is implicit. Using the identity $1/x^+ = -i\int_0^t dt\, e^{ix^+t}$, and representing the trace $\mathrm{tr}\,\hat{A} = \int dq\langle q|\hat{A}|q\rangle$ as a real space integral,

$$\rho(\epsilon) = \frac{1}{\pi\hbar}\int_0^\infty dt\,\mathrm{Re}\,\mathrm{tr}(e^{i(\epsilon^+-\hat{H})t/\hbar}) = \frac{1}{\pi}\,\mathrm{Re}\int_0^\infty dt\, e^{i\epsilon^+t/\hbar}\int dq\langle q|e^{-i\hat{H}t/\hbar}|q\rangle\,, \tag{3.59}$$

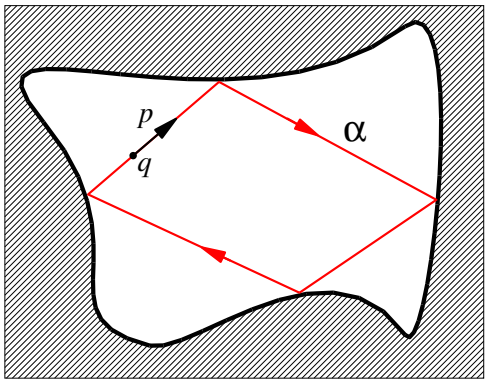
we have made the connection between the density of states and the quantum propagation amplitude explicit.

Without going into full mathematical detail (see, for example, Ref. [**?**] for a modern discourse) we now outline how this integral is evaluated by path integral techniques within the semiclassical approximation. Although, for brevity, some of the more tricky steps of the calculation are swept unter the carpet, the sketch will be accurate enough to make manifest some aesthetic connections between the spectral theory of chaotic quantum systems and classically chaotic dynamics. (For a more formal and thorough discussion, we refer to Gutzwiller and Haake.)

Making use of the semiclassical approximation (3.28) established earlier, when substituted into Eq. (3.59), one obtains $\rho(\epsilon) \simeq \frac{1}{\pi}\,\mathrm{Re}\int_0^\infty dt\, e^{i\epsilon^+t/\hbar}\int dq\, A[q_{\rm cl}]e^{\frac{i}{\hbar}S[q_{\rm cl}]}$, where, following our discussion in section 3.2.2, we have defined $A[q_{\rm cl}] \equiv \det\left(\frac{i}{2\pi\hbar}\frac{\partial^2 S[q_{\rm cl}]}{\partial q(0)\partial q(t)}\right)^{1/2}$ and $q_{\rm cl}$ represents a closed classical path that begins at q at time zero and ends at the same coordinate at time t. Again relying on the semiclassical condition $S[q_{\rm cl}] \gg \hbar$, the integrals over q and t can be performed in a stationary phase approximation. Beginning with the time integral, and noticing that $\partial_t S[q_{\rm cl}] = -\epsilon_{q_{\rm cl}}$ is the (conserved) energy of the path $q_{\rm cl}$, we obtain the saddle point condition $\epsilon \stackrel{!}{=} \epsilon_{q_{\rm cl}}$ and

$$\rho(\epsilon) \simeq \frac{1}{\pi}\,\mathrm{Re}\int dq\, A[q_{{\rm cl},\epsilon}]e^{\frac{i}{\hbar}S[q_{{\rm cl},\epsilon}]}\,,$$

where the symbol $q_{{\rm cl},\epsilon}$ indicates that only paths $q\to q$ of energy ϵ are taken into account, and the contribution coming from the quadratic integration around the saddle point has been absorbed into a redefinition of $A[q_{{\rm cl},\epsilon}]$.



Turning to the q–integration, making use of the fact that $\partial_{q_i}S[q_{\rm cl}] = -p_i$, $\partial_{q_f}S[q_{\rm cl}] = p_f$, where $q_{i,f}$ are the initial and final coordinate of a path $q_{\rm cl}$, and $p_{i,f}$ are the initial and final momentum, the stationary phase condition assumes the form $0 \stackrel{!}{=} d_q S[q_{{\rm cl},\epsilon}] = \left(\partial_{q_i}+\partial_{q_f}\right)S[q_{{\rm cl},\epsilon}]|_{q_i=q_f=q} = p_f - p_i$, i.e. the stationarity of the integrand under the q–integration requires the initial and final momentum of the path $q_{{\rm cl},\epsilon}$ be identical. We thus find that the paths contributing to the integrated transition amplitude are not only periodic in coordinate space but even in phase space. Such paths are called **periodic orbits** —'periodic' because the path comes back to its initial

phase space coordinate after a certain revolution time. As such, the orbit will be traversed repeatedly as time goes by (see the figure, where a periodic orbit α with initial coordinates $x = (p, q)$ is shown).

According to our analysis above, each coordinate point q lying on a periodic orbit is a stationary phase point of the q–integral. The stationary phase approximation of the integral can thus be formulated as

$$\rho(\epsilon) \simeq \frac{1}{\pi} \mathrm{Re} \int dq\, A[q_{\mathrm{cl},\epsilon}] e^{\frac{i}{\hbar} S[q_{\mathrm{cl},\epsilon}]} \simeq \sum_{n=1}^{\infty} \sum_{\alpha} \int_{\alpha} dq\, A_\alpha e^{\frac{i}{\hbar} n S_\alpha},$$

where $\sum_\alpha$ stands for a sum over all periodic orbits (of energy ϵ) and S_α is the action corresponding to one traversal of the orbit (all at fixed energy ϵ). The index n accounts for the fact that, due to its periodicty, the orbit can be traversed repeatedly, with total action nS_α. Furthermore, $\int_\alpha dq$ is an integral over all coordinates lying on the orbit and we have again absorbed a contribution coming from the quadratic integration around the stationary phase points in the pre–exponential amplitude A_α.

Finally, noting that $\int_\alpha dq \propto T_\alpha$, where T_α is the period of one traversal of the orbit α (at energy ϵ), we arrive at the result

$$\boxed{\rho(\epsilon) \simeq \frac{1}{\pi} \mathrm{Re} \sum_{n=1}^{\infty} \sum_{\alpha} T_\alpha\, A_\alpha e^{\frac{i}{\hbar} n S_\alpha}} \tag{3.60}$$

This is (a simplified[41]) representation of the famous **Gutzwiller trace formula**. The result is actually quite remarkable: The density of states, an observable of quantum mechanical signifi-

[41] Had we carefully kept track of all determinants arising from the stationary phase integrals, the prefactor A_α would have read

$$A_\alpha = \frac{1}{\hbar} \frac{e^{i\frac{\pi}{2}\nu_\alpha}}{|\det M_\alpha^r - 1|^{\frac{1}{2}}},$$

where ν_α is known as the **Maslov index** (an integer valued factor associated with the singular points on the orbit, i.e. the classical turning points). The meaning of this object can be understood, e.g., by applying the path integral to the problem of a quantum particle in a box. To correctly reproduce the spectrum, the contribution of each path must be weighted by $(-)^n = \exp(i\pi n)$, where n is the number of its turning points in the box potential), and M_α represents the **Monodromy matrix**. To understand the meaning of this object, notice that a phase space point $\bar{x}$ on a periodic orbit can be interpreted as a fixed point of the *classical* time evolution operator $U(T_\alpha)$: $U(T_\alpha, \bar{x}) = \bar{x}$, which is just to say that the orbit is periodic. As with any other smooth mapping, U can be linearized in the vicinity of its fixed points, $U(T_\alpha, \bar{x} + y) = \bar{x} + M_\alpha y$, where the linear operator M_α is the monodromy matrix. Evidently, M_α determines the stability of the orbit under small distortions, which makes it plausible that it appears as a controlling prefactor of the stationary phase approximation to the density of states.

▷ Exercise. Making use of the Feynman path integral, show that the propagator for a particle of mass m confined by a square well potential of infinite strength is given by

$$G(q_F, q_I; t) = \sqrt{\frac{m}{2\pi i\hbar t}} \sum_{n=-\infty}^{\infty} \left\{ \exp\left[\frac{im(q_F - q_I + 2na)^2}{2\hbar t}\right] - \exp\left[\frac{im(q_F + q_I + 2na)^2}{2\hbar t}\right] \right\}.$$

cance, has been expressed entirely in terms of classical quantities.

3.4 Summary

In this chapter we have introduced the path integral formulation of quantum mechanics, an approach independent of, yet (modulo certain mathematical imponderabilities related to continuum functional integration) equivalent to the standard route of canonical operator quantization. While a few precious exactly solvable quantum problems (e.g. the evolution of a free particle, the harmonic oscillator, and, perhaps intriguingly, quantum mechanical spin) are more efficiently formulated by the standard approach, a spectrum of unique features make the path integral an indispensible tool of modern quantum mechanics: The path integral approach is highly intuitive, powerful in the treatment of non-perturbative problems, and tailor–made to formulation of semiclassical limits. Perhaps most importantly, we have seen that it provides a unifying link whereby quantum problems can be related to classical statistical mechanics. Indeed, we have found that the path integral of a quantum point particle is, in many respects, equivalent to the partition function of a classical one–dimensional continuum system. We have hinted at a generalization of this prinicple, i.e. an equivalence priniciple relating d–dimensional quantum *field* theory to $d+1$–dimensional statistical mechanics. However, before exploring this bridge further, we first need to generalize the concept of path integration to problems involving quantum fields. This will be the subject of the next chapter.

Chapter 4

Functional Field Integral

In this chapter, the concept of path integration is generalized to integration over quantum fields. Specifically we will develop an approach to quantum field theory that takes as its starting point an integration over all configurations of a given field, weighted by an appropriate action. To emphasize the importance of the formulation which, methodologically, represents the backbone of the remainder of the text, we have pruned the discussion to focus only on the essential elements. This being so, conceptual aspects stand in the foreground and the discussion of applications is postponed to the following chapters.

In this chapter, the concept of path integration will be extended from quantum mechanics to quantum field theory. Our starting point will be from a situation very much analogous to that outlined at the beginning of the previous chapter. Just as there are two different approaches to quantum mechanics, quantum field theory can also be formulated in two different ways; the formalism of canonically quantised field operators, and functional integration. As for the former, although much of the technology needed to efficiently implement this framework — essentially Feynman diagrams — originated in high energy physics, it was with the development of condensed matter physics through the 50s, 60s and 70s that this approach was driven to unprecedented sophistication. The reason is that, almost as a rule, problems in condensed matter investigated at that time necessitated perturbative summations to *infinite* order in the non–trivial content of the theory (typically interactions). This requirement led to the development of advanced techniques to sum (subsets of) the perturbation series in many–body interaction operators to infinite order.

In the 70s, however, essentially *non–perturbative* problems began to attract more and more attention — a still prevailing trend — and it turned out that the formalism of canonically quantised operators was not tailored to this type of physics. By contrast, the alternative approach to many–body problems, functional integration, is ideally suited! The situation is similar to the one described in the last chapter where we saw that the Feynman path integral provided an entire spectrum of novel routes to approaching quantum mechanical problems (controlled semi–classical limits, analogies to classical mechanics, statistical mechanics, concepts of topology and geometry, etc.). Similarly, the introduction of functional field integration into many–body physics spawned plenty of new theoretical developments, many of which were manifestly non–perturbative. Moreover, the advantages of the path integral approach in many–body physics is even more

pronounced than in single particle quantum mechanics. Higher dimensionality introduces fields of a more complex internal structure allowing for non–trivial topology while, at the same time, the connections to classical statistical mechanics play a much more important role than in single particle quantum mechanics.

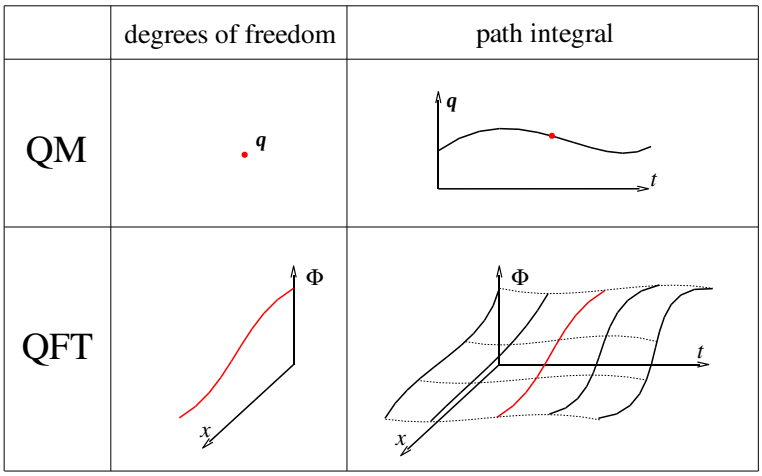


Figure 4.1: The concept of field integration. Upper panels: path integral of quantum mechanics — integration over all time-dependent configurations of a point particle degree of freedom leads to integrals over *curves*. Lower panels: field integral — integration over time dependent configurations of d–dimensional continuum mappings (fields) leads to integrals over generalized $(d+1)$–dimensional *surfaces*.

All of these concepts will begin to play a role in subsequent chapters when applications of the field integral are discussed. Before embarking on the quantitative construction — the subject of the following sections — let us first anticipate the kind of structures that one should expect. In quantum mechanics, we were starting from a single point particle degree of freedom, characterized by some coordinate $\mathbf{q}$ (or some other quantum numbers for that matter). Path integration then meant integration over all time–dependent configurations $\mathbf{q}(t)$, i.e. a set of *curves* $t \mapsto \mathbf{q}(t)$ (see Fig. 4.1 upper panel). By contrast, the degrees of freedom of field theory are continuous objects $\Phi(x)$ by themselves, where x parameterizes some d–dimensional base manifold and Φ takes values in some target manifold (Fig. 4.1, lower panel). The natural generalization of a 'path' integral then implies integration over a single copy of these objects at each instant of time, i.e. we shall have to integrate over generalized *surfaces*, mappings from $(d+1)$–dimensional space–time into the field manifold, $(x,t) \mapsto \Phi(x,t)$. While this notion may sound worrying, it is important to realize that, conceptually, nothing much changes in comparison with the path integral: instead of a one–dimensional manifold — a curve — our object of integration will be a $(d+1)$–dimensional manifold.

We now proceed to formulate these ideas in quantitative terms.

▷ Exercise. If necessary, recapitulate the general construction scheme of path integrals (section 3.2.3) and the connection between quantum fields and second quantized operators.

4.1 Construction of the Many–body Path Integral

The construction of a path integral for field operators follows the general scheme outlined at the end of section 3.2.3. The basic idea is to segment the time evolution of a quantum (many–body) Hamiltonian into infinitesimal time slices and to absorb as much as is possible of the quantum dynamical phase accumulated during the short time propagation into a set of suitably chosen eigenstates. But how should these eigenstates be chosen? In the context of single particle quantum mechanics, the basic structure of the Hamiltonian suggested the choice of a representation in terms of coordinate and momentum eigenstates. Now, given that many particle Hamiltonians are conveniently expressed in terms of creation/annihilation operators, an obvious idea would be to search for eigenstates of *these* operators. Such states indeed exist and are called **coherent states**.

4.1.1 Coherent States (Bosons)

Our goal is, therefore, to find eigenstates of the Fock space (non–Hermitian) operators $a^\dagger$ and a. Although the general form of these states will turn out to be the same for bosons and fermions, there are major differences regarding their algebraic structure. The point is that the anticommutation relations of fermions require that the eigenvalues of an annihilation operator themselves anticommute, i.e. they *cannot* be ordinary numbers. Postponing the introduction of the unfamiliar concept of anticommuting 'numbers' to the next section, we first concentrate on the bosonic case where problems of this kind do not arise.

So what form do the eigenstates $|\phi\rangle$ of the bosonic Fock space operators a, and $a^\dagger$ take? Being a state of the Fock space, an eigenstate $|\phi\rangle$ can be expanded as

$$|\phi\rangle = \sum_{n_1,n_2,\cdots} C_{n_1,n_2,\cdots}|n_1,n_2\cdots\rangle, \qquad |n_1,n_2\cdots\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1}}\frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2}}\cdots|0\rangle\,,$$

where $a_i^\dagger$ creates a boson in state i, $C_{n_1,n_2,\cdots}$ represents a set of expansion coefficients, and $|0\rangle$ represents the vacuum. Here, for reasons of clarity, it is convenient to adopt this convention for the vacuum as opposed to the notation $|\Omega\rangle$ used previously. Furthermore, the many–body state $|n_1,n_2\cdots\rangle$ is indexed by a set of occupation numbers: n_1 in state $|1\rangle$, n_2 in state $|2\rangle$, and so on. Importantly, the state $|\phi\rangle$ can, in principle (and will in practice) contain a superposition of basis states which have different numbers of particles. Now, if the minimum number of particles in state $|\phi\rangle$ is n_0, the minimum of $a_i^\dagger|\phi\rangle$ must be n_0+1: Clearly the *creation* operators $a_i^\dagger$ themselves cannot possess eigenstates.

However, with annihilation operators this problem does not arise. Indeed, the annihilation operators do possess eigenstates known as **bosonic coherent states**

$$\boxed{|\phi\rangle \equiv \exp\left[\sum_i \phi_i a_i^\dagger\right]|0\rangle} \tag{4.1}$$

where the elements of $\phi = \{\phi_i\}$ represent a set of complex numbers. The states $|\phi\rangle$ are

eigenstates in the sense that, for all i,

$$\boxed{a_i|\phi\rangle = \phi_i|\phi\rangle} \tag{4.2}$$

i.e. they simultaneously diagonalise all annihilation operators. Noting that a_i and $a_j^\dagger$, with $j \neq i$, commute, Eq. (4.2) can be verified by showing that $a\exp(\phi a^\dagger)|0\rangle = \phi\exp(\phi a^\dagger)|0\rangle$.[1] Although not crucial to the practice of functional field integration, in the construction of the many–body path integral, it will be useful to assimilate some further properties of coherent states.

▷ By taking the Hermitian conjugate of Eq. (4.2), we find that the 'bra' associated with the 'ket' $|\phi\rangle$ is a left eigenstate of the set of creation operators, i.e. for all i,

$$\langle\phi|a_i^\dagger = \langle\phi|\bar{\phi}_i \tag{4.3}$$

where $\bar{\phi}_i$ is the complex conjugate of ϕ_i, and $\langle\phi| = \langle 0|\exp[\sum_i \bar{\phi}_i a_i]$.

▷ It is a straightforward matter — e.g. by a Taylor expansion of Eq. (4.1) — to show that the action of a creation operator on a coherent state yields the identity

$$a_i^\dagger|\phi\rangle = \partial_{\phi_i}|\phi\rangle. \tag{4.4}$$

Reassuringly, it may be confirmed that Eqs. (4.4) and (4.2) are consistent with the commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$: $[a_i, a_j^\dagger]|\phi\rangle = (\partial_{\phi_j}\phi_i - \phi_i\partial_{\phi_j})|\phi\rangle = \delta_{ij}|\phi\rangle$.

▷ Making use of the relation $\langle\theta|\phi\rangle = \langle 0|e^{\sum_i \bar{\theta}_i a_i}|\phi\rangle = e^{\sum_i \bar{\theta}_i\phi_i}\langle 0|\phi\rangle$ one finds that the overlap between two coherent states is given by

$$\langle\theta|\phi\rangle = \exp\left[\sum_i \bar{\theta}_i\phi_i\right] \tag{4.5}$$

▷ From this result, one can infer that the norm of a coherent state is given by

$$\langle\phi|\phi\rangle = \exp\left[\sum_i \bar{\phi}_i\phi_i\right] \tag{4.6}$$

▷ Most importantly, the coherent states form a complete — in fact an overcomplete — set of states in Fock space:

$$\boxed{\int\prod_i \frac{d\bar{\phi}_i d\phi_i}{\pi} e^{-\sum_i \bar{\phi}_i\phi_i}|\phi\rangle\langle\phi| = \mathbf{1}_{\mathcal{F}},} \tag{4.7}$$

where $d\bar{\phi}_i d\phi_i = d\mathrm{Re}\,\phi_i d\mathrm{Im}\,\phi_i$, and $\mathbf{1}_{\mathcal{F}}$ represents the unit operator or identity in the Fock space.

[1] Using the result $[a,(a^\dagger)^n] = n(a^\dagger)^{n-1}$ (cf. Eq. **??**) a Taylor expansion shows $a\exp(\phi a^\dagger)|0\rangle = [a,\exp(\phi a^\dagger)]|0\rangle = \sum_{n=0}^\infty \frac{\phi^n}{n!}[a,(a^\dagger)^n]|0\rangle = \sum_{n=1}^\infty \frac{n\phi^n}{n!}(a^\dagger)^{n-1}|0\rangle = \phi\sum_{n=1}^\infty \frac{\phi^{n-1}}{(n-1)!}(a^\dagger)^{n-1}|0\rangle = \phi\exp(\phi a^\dagger)|0\rangle$.

▷ INFO. The proof of Eq. (4.7) proceeds by straightforward application of Schur's lemma (cf. our discussion of the completeness of the spin coherent states in the previous chapter): The operator family $\{a_i\}$, $\{a_i^\dagger\}$ acts irreducibly in Fock space. According to Schur's lemma, the proportionality of the left hand side of Eq. (4.7) to the unit operator is, therefore, equivalent to its commutativity with all creation and annihilation operators. Indeed, this property is easily confirmed:

$$a_i \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i} |\phi\rangle\langle\phi| = \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i} \phi_i |\phi\rangle\langle\phi| = -\int d(\bar{\phi},\phi) \left(\partial_{\bar{\phi}_i} e^{-\sum_i \bar{\phi}_i\phi_i}\right) |\phi\rangle\langle\phi|$$
$$\overset{\text{by parts}}{=} \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i} |\phi\rangle \left(\partial_{\bar{\phi}_i}\langle\phi|\right) = \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i} |\phi\rangle\langle\phi| a_i, \tag{4.8}$$

where, for brevity, we have set $d(\bar{\phi},\phi) \equiv \prod_i d\bar{\phi}_i d\phi_i/\pi$. Taking the adjoint of Eq. (4.8), one may further check that the left hand side of (4.7) commutes with the set of creation operators, i.e. it must be proportional to the unit operator. To fix the constant of proportionality, one may simply take the overlap with the vacuum:

$$\int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i} \langle 0|\phi\rangle\langle\phi|0\rangle = \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i} = 1, \tag{4.9}$$

where the last equality follows from Eq. (3.11). Taken together, Eqs. (4.8) and (4.9) prove (4.7). Note that the coherent states are overcomplete in the sense that they are not mutually orthogonal (see Eq. (4.5)). The exponential weight $e^{-\sum_i \bar{\phi}_i\phi_i}$ appearing in the resolution of the identity compensates for the overcounting achieved by integrating over the whole set of coherent states.

With these definitions we have all that we need to construct the many–body path integral for the bosonic system. However, before doing so, we will first introduce the fermionic version of the coherent state. This will allow us to construct the path integrals for bosons and fermions simultaneously, thereby emphasising the similarity of their structure.

4.1.2 Coherent States (Fermions)

Surprisingly, much of the formalism above generalises to the fermionic case: As before, it is evident that creation operators cannot possess eigenstates. Following the bosonic system, let us suppose that the annihilation operators are characterised by a set of coherent states such that, for all i,

$$\boxed{a_i|\eta\rangle = \eta_i|\eta\rangle} \tag{4.10}$$

where η_i is the eigenvalue. Although the structure of this equation appears to be equivalent to its bosonic counterpart (4.2) it has one frustrating feature: Anticommutativity of the fermionic operators, $[a_i, a_j]_+ = 0$, where $i \neq j$, implies that the eigenvalues η_i also have to anticommute,

$$\boxed{\eta_i\eta_j = -\eta_j\eta_i} \tag{4.11}$$

Clearly, these objects cannot be ordinary numbers. In order to define a fermionic version of coherent states, we now have two choices: We may (a) accept Eq.(4.11) as a working

definition and pragmatically explore its consequences, or (b), first try to remove any mystery from the definitions (4.10) and (4.11). This latter task is tackled in the info block below where objects $\{\eta_i\}$ with the desired properties are defined in a mathematically consistent manner. Readers wishing to proceed in a maximally streamlined manner may skip this exposition and directly turn to the more praxis–oriented discussion below.

▷ INFO. There is a mathematical structure ideally suited to generalize the concept of ordinary number(fields), namely **algebras**. An algebra $\mathcal{A}$ is a vector space endowed with a multiplication rule $\mathcal{A} \times \mathcal{A} \to \mathcal{A}$. So, let us *construct* an algebra $\mathcal{A}$ by starting out from a set of elements, or generators, $\eta_i \in \mathcal{A}, i = 1, \ldots N$, and imposing the rules:

(i) The elements η_i can be added and multiplied by complex numbers, viz.

$$c_0 + c_i\eta_i + c_j\eta_j, \in \mathcal{A} \quad c_0, c_i, c_j \in \mathbb{C}\,, \tag{4.12}$$

i.e. $\mathcal{A}$ is a complex vectorspace.

(ii) The product, $\mathcal{A} \times \mathcal{A} \to \mathcal{A}, (\eta_i, \eta_j) \mapsto \eta_i\eta_j$, is associative and anticommutative, i.e. it obeys the anti–commutation relation (4.11). Because of the associativity of this operation, there is no ambiguity when it comes to forming products of higher order, i.e. $(\eta_i\eta_j)\eta_k = \eta_i(\eta_j\eta_k) \equiv \eta_i\eta_j\eta_k$. The definition requires that products of odd order in the number of generators anti–commute, while (even,even) and (even,odd) combinations commute (exercise).

By virtue of (i) and (ii), the set $\mathcal{A}$ of all linear combinations $c_0 + \sum_{n=1}^{\infty} \sum_{i_1,\cdots i_n=1}^{N} c_{i_1,\ldots,i_n}\eta_{i_1} \ldots \eta_{i_n}$, $c_0, c_{i_1,\ldots,i_n} \in \mathbb{C}$ spans a finite–dimensional associative algebra $\mathcal{A}$,[2] known as the **Grassmann algebra**[3] (and sometimes also the **exterior algebra**).

For completeness we mention that Grassmann algebras find a number of realizations in mathematics, the most basic being exterior multiplication in linear algabra: Given an N–dimensional vector space V, let V^* be the dual space, i.e. the space of all linear mappings, or 'forms' $\Lambda : V \to \mathbb{C}, v \mapsto \Lambda(v)$, where $v \in V$. (Like V, V^* is a vector space of dimension N.) Next, define exterior multiplication through, $(\Lambda, \Lambda') \to \Lambda \wedge \Lambda'$, where $\Lambda \wedge \Lambda'$ is the mapping

$$\begin{aligned} \Lambda \wedge \Lambda' : V \times V &\to \mathbb{C} \\ (v, v') &\mapsto \Lambda(v)\Lambda'(v') - \Lambda(v')\Lambda'(v). \end{aligned}$$

This operation is manifestly anti–commutative: $\Lambda \wedge \Lambda' = -\Lambda \wedge \Lambda'$. Identifying the N linear basis forms $\Lambda_i \leftrightarrow \eta_i$ with generators and $\wedge$ with the product, we see that the space of exterior forms of a vector space forms a Grassmann algebra.

---

[2] ...whose dimension can be shown to be 2^N (exercise)

Hermann Günter Grassmann 1809–1877: credited for inventing what is now called Exterior Algebra.

[3]

Apart from their anomalous commutation properties, the generators $\{\eta_i\}$, and their product generalizations $\{\eta_i\eta_j, \eta_i\eta_j\eta_k, \ldots\}$ resemble ordinary, albeit anti-commutative numbers. (In practice, the algebraic structure underlying their definition can safely be ignored. All we will need to work with these objects is the basic rule (4.11) and the property (4.12).) We emphasize that $\mathcal{A}$ not only contains anticommuting but also commuting elements, i.e. linear combinations of an *even* number of Grassmann numbers η_i are overall commutative. (This mimics the behaviour of the Fock space algebra: products of an even number of annihilation operators $a_i a_j \ldots$ commute with all other linear combinations of operators a_i. In spite of this similarity, the 'numbers' η_i must not be confused with the Fock space operators; there is nothing on which they act.)

To make practical use of the new concept, we need to go beyond the level of pure arithmetic. Specifically, we need to introduce functions of anti–commuting numbers, and elements of calculus. Remarkably, most of the concepts of calculus not only naturally generalize to anti–commuting number fields, but contrary to what one might expect, the anti–commutative generalization of differentiation, integration, etc. turns out to be much *simpler* than in ordinary calculus.

▷ Functions of Grassmann numbers are defined via their Taylor expansion:

$$\xi_1, \ldots, \xi_k \in \mathcal{A}: \qquad f(\xi_1, \ldots, \xi_k) = \sum_{n=0}^{\infty} \sum_{i_1, \cdots i_n = 1}^{k} \frac{1}{n!} \frac{\partial^n f}{\partial \xi_{i_1} \ldots \partial \xi_{i_n}}\Big|_{\xi=0} \xi_{i_n} \ldots \xi_{i_1}, \quad (4.13)$$

where f is an analytic function. Note that the anticommutation properties of the algebra implies that the series terminates after a *finite* number of terms. For example, in the simple case where η is first order in the generators of the algebra, $N = 1$, and $f(\eta) = f(0) + f'(0)\eta$ (since $\eta^2 = 0$).

▷ Differentiation with respect to Grassmann numbers is defined by

$$\boxed{\partial_{\eta_i} \eta_j = \delta_{ij}} \quad (4.14)$$

Note that in order to be consistent with the commutation relations, the differential operator ∂_{η_i} must itself be anti–commutative. In particular, $\partial_{\eta_i}\eta_j\eta_i \stackrel{i\neq j}{=} -\eta_j$.

▷ Integration over Grassmann variables is defined by

$$\boxed{\int d\eta_i = 0, \qquad \int d\eta_i \eta_i = 1} \quad (4.15)$$

Note that the definitions (4.13), (4.14) and (4.15) imply that the action of *Grassmann differentiation and integration are effectively identical*, viz.

$$\int d\eta f(\eta) = \int d\eta (f(0) + f'(0)\eta) = f'(0) = \partial_\eta f(\eta)\,.$$

With this background, let us now proceed to apply the Grassmann algebra to the construction of fermion coherent states. To this end we need to enlarge the algebra even further so as to allow for a multiplication of Grassmann numbers by fermion operators. In order to be consistent with the anticommutation relations, we need to require that fermion operators and Grassmann generators anticommute,

$$[\eta_i, a_j]_+ = 0\,. \tag{4.16}$$

It then becomes a straightforward matter to demonstrate that **fermionic coherent states** are defined by

$$\boxed{|\eta\rangle = \exp\left[-\sum_i \eta_i a_i^\dagger\right]|0\rangle} \tag{4.17}$$

i.e. by a structure perfectly analogous to the bosonic states (4.1).[4] It is a straightforward matter — and also a good exercise — to demonstrate that the properties (4.3), (4.4), (4.5), (4.6) and, most importantly, (4.7) carry over to the fermionic case. One merely has to identify a_i with a fermionic operator and replace the complex variables ϕ_i by $\eta_i \in \mathcal{A}$. Apart from a few sign changes and the $\mathcal{A}$–valued arguments, the fermionic coherent states differ only in two respects from their bosonic counterpart: firstly, the Grassmann variables $\bar\eta_i$ appearing in the adjoint of a fermion coherent state,

$$\langle\eta| = \langle 0|\exp\left[-\sum_i a_i\bar\eta_i\right] = \langle 0|\exp\left[\sum_i \bar\eta_i a_i\right]\,,$$

are *not* related to the η_is of the state $|\eta\rangle$ via some kind of complex conjugation. Rather η_i and $\bar\eta_i$ are strictly independent variables.[5] Secondly, the Grassmann version of a Gaussian integral (exercise), $\int d\bar\eta d\eta\, e^{-\bar\eta\eta} = 1$ does not contain the factors of π characteristic of standard Gaussian integrals. Thus, the measure of the fermionic analogue of Eq. (4.7) does not contain a π in the denominator.

For the sake of future reference, the most important properties of Fock space coherent states are summarised in table 4.1.

[4] To prove that the states (4.17) indeed fulfil the defining relation (4.10), we note that $a_i\exp(-\eta_i a_i^\dagger)|0\rangle \overset{(4.13)}{=} a_i(1-\eta_i a_i^\dagger)|0\rangle \overset{(4.16)}{=} \eta_i a_i a_i^\dagger|0\rangle = \eta_i|0\rangle = \eta_i(1-\eta_i a_i^\dagger)|0\rangle = \eta_i\exp(-\eta_i a_i^\dagger)|0\rangle$. This, in combination with the fact that a_i and $\eta_j a_j^\dagger$ $(i \neq j)$ commute proves (4.10). Note that the proof has actually been simpler than in the bosonic case. The fermionic Taylor series terminates after the first contribution. This observation is representative of a general rule: Grassmann calculus is simpler than standard calculus; all series are finite, integrals always converge, etc.

[5] In the literature, complex conjugation of Grassmann variables is sometimes defined. Although appealing from an aesthetic point of view — symmetry between bosons and fermions — this concept is problematic. The difficulties become apparent when **supersymmetric theories** are considered, i.e. theories where operator algebras contain both bosons and fermions (the so–called super–algebras). It is not possible to introduce a complex conjugation that leads to compatibility with the commutation relations of a super–algebra. It therefore seems to be better to abandon the concept of Grassmann complex conjugation altogether. Note that although, in the bosonic case, complex conjugation is inevitable (in order to define convergent Gaussian integrals, say), no such need arises in the fermionic case.

Definition	$\|\psi\rangle = \exp\left[\zeta \sum_i \psi_i a_i^\dagger\right] \|0\rangle$
Action of a_i	$a_i\|\psi\rangle = \psi_i\|\psi\rangle, \qquad \langle\psi\|a_i = \partial_{\bar\psi_i}\langle\psi\|$
Action of $a_i^\dagger$	$a_i^\dagger\|\psi\rangle = \zeta\partial_{\psi_i}\|\psi\rangle, \qquad \langle\psi\|a_i^\dagger = \langle\psi\|\bar\psi_i$
Overlap	$\langle\psi'\|\psi\rangle = \exp\left[\sum_i \bar\psi_i'\psi_i\right]$
Completeness	$\int d(\bar\psi,\psi)\, e^{-\sum_i \bar\psi_i\psi_i}\|\psi\rangle\langle\psi\| = \mathbf{1}_{\mathcal{F}}$

Table 4.1: Basic properties of coherent states for bosons ($\zeta = 1$, $\psi_i \in \mathbb{C}$) and fermions ($\zeta = -1$, $\psi_i \in \mathcal{A}$). In the last line, the integration measure is defined as $d(\bar\psi,\psi) \equiv \prod_i \frac{d\bar\psi_i d\psi_i}{\pi^{(1+\zeta)/2}}$.

▷ INFO. **Grassmann Gaussian Integration:** Finally, before turning to the development of the functional field integral, it is useful to digress on the generalization of higher dimensional Gaussian integrals for Grassmann variables. The prototype of all Grassmann Gaussian integration formulae is the identity

$$\boxed{\int d\bar\eta d\eta\, e^{-\bar\eta a\eta} = a} \tag{4.18}$$

where $a \in \mathbb{C}$ takes arbitrary values. Eq. (4.18) is derived by a first order Taylor expansion of the exponential and application of Eq. (4.15). The multi–dimensional generalization of (4.18) is given by

$$\int d(\bar\phi,\phi) e^{-\bar\phi^T \mathbf{A}\phi} = \det \mathbf{A}\,, \tag{4.19}$$

where $\bar\phi$ and ϕ are N–component vectors of Grassmann variables, the measure $d(\bar\phi,\phi) \equiv \prod_{i=1}^N d\bar\phi_i d\phi_i$, and $\mathbf{A}$ may be an *arbitrary* complex matrix. For matrices that are unitarily diagonalisable, $\mathbf{A} = \mathbf{U}^\dagger\mathbf{D}\mathbf{U}$, with $\mathbf{U}$ unitary, and $\mathbf{D}$ diagonal, Eq. (4.19) is proven in the same way as its complex counterpart (3.17): One changes variables $\phi \to \mathbf{U}^\dagger\phi$, $\bar\phi \to \mathbf{U}^T\bar\phi$. Since $\det \mathbf{U} = 1$, the transform leaves the measure invariant (see below) and leaves us with N decoupled integrals of the type (4.18). The resulting product of N eigenvalues is just the determinant of $\mathbf{A}$ (cf. the later discussion of the partition function of the non–interacting gas). For general (non–diagonalisable) $\mathbf{A}$, the identity is established by a straightforward expansion of the exponent. The expansion terminates at Nth order and, by commuting through integration variables, it may

be shown that the resulting Nth order polynomial of matrix elements of $\mathbf{A}$ is the determinant.[6]

Keeping the analogy with ordinary commuting variables, the Grassmann version of Eq. (3.18) reads

$$\int d(\bar{\phi},\phi) e^{-\bar{\phi}^T \mathbf{A}\phi + \bar{\nu}^T\cdot\phi + \bar{\phi}^T\cdot\nu} = e^{\bar{\nu}^T \mathbf{A}^{-1}\nu} \det \mathbf{A} \tag{4.22}$$

To prove the latter, we note that $\int d\eta f(\eta) = \int d\eta f(\eta+\nu)$, i.e. in Grassmann integration one can shift variables as in the ordinary case. The proof of the Gaussian relation above thus proceeds in complete analogy to the complex case. As with Eq. (3.18), Eq. (4.22) can also be employed to generate further integration formulae. Defining $\langle\cdots\rangle \equiv \det \mathbf{A}^{-1} \int d(\bar{\phi},\phi) e^{-\bar{\phi}^T\mathbf{A}\phi}(\cdots)$, and expanding both the left and the right hand side of (4.22) to leading order in the 'monomial' $\bar{\nu}_j\nu_i$, one obtains $\langle \eta_j \bar{\eta}_i\rangle = A^{-1}_{ji}$. Finally, the N–fold iteration of this procedure gives

$$\boxed{\langle \eta_{j_1}\eta_{j_2}\ldots\eta_{j_n}\bar{\eta}_{i_1}\bar{\eta}_{i_2}\ldots\bar{\eta}_{i_n}\rangle = \sum_P (\text{ sgn } P)\, A^{-1}_{j_1 i_{P_1}}\ldots A^{-1}_{j_n i_{P_n}}}$$

where the signum of the permutation accounts for the sign changes accompanying the interchange of Grassmann variables. Finally, as with Gaussian integration over commuting variables, by taking $N\to\infty$, the Grassmann integration can be translated to a Gaussian functional integral.

4.2 Field Integral for the Quantum Partition Function

Having introduced the coherent states, we will see that the construction of path integrals for many–body systems no longer presents substantial difficulties. However, be-

[6] As with ordinary integrals, Grassmann integrals can also be subjected to **variable transforms**. Suppose we are given an integral $\int d(\bar{\phi},\phi) f(\bar{\phi},\phi)$ and wish to change variables according to

$$\bar{\nu} = \mathbf{M}\bar{\phi}, \quad \nu = \mathbf{M}'\phi\,, \tag{4.20}$$

where, for simplicity, $\mathbf{M}$ and $\mathbf{M}'$ are complex matrices (i.e. we here restrict ourselves to linear transforms). One can show that

$$\bar{\nu}_1\ldots\bar{\nu}_N = (\det\mathbf{M})\bar{\phi}_1\ldots\bar{\phi}_N, \qquad \nu_1\ldots\nu_N = (\det\mathbf{M}')\phi_1\ldots\phi_N\,. \tag{4.21}$$

(There are different ways to prove this identity. The most straightforward is by explicitly expanding (4.20) in components and commuting all Grassmann variables to the right. A more elegant way is to argue that the coefficient relating the right and the left hand sides of (4.21) must be an Nth order polynomial of matrix elements of $\mathbf{M}$. In order to be consistent with the anti–commutation behaviour of Grassmann variables, the polynomial must obey commutation relations which uniquely characterise a determinant. Excercise: Check the relation for $N=2$.) On the other hand, the integral of the new variables must obey the defining relation, $\int d\bar{\nu}\bar{\nu}_1\ldots\bar{\nu}_N = \int d\nu\nu_1\ldots\nu_N = (-)^{N+1}$, where $d\bar{\nu} = \prod_{i=1}^N d\bar{\nu}_i$ and the sign on the right hand side is attributed to ordering of the integrand, viz. $\int d\nu_1 d\nu_2 \nu_1\nu_2 = -\int d\nu_1\nu_1 \int d\nu_2\nu_2 = -1$. Together Eqs. (4.21) and (4.20) enforce the identities $d\bar{\nu} = (\det\mathbf{M})^{-1} d\bar{\phi}$, $d\nu = (\det\mathbf{M}')^{-1}d\phi$, which combine to give

$$\int d(\bar{\phi},\phi) f(\bar{\phi},\phi) = \det(\mathbf{M}\mathbf{M}') \int d(\bar{\nu},\nu') f(\bar{\phi}(\bar{\nu}),\phi(\nu))\,.$$

fore proceeding, we should address the question; what does the phrase 'path–integral for many–body systems' actually mean? In the next chapter we will see that much of the information about a quantum many–particle systems is encoded in expectation values of products of creation and annihilation operators, i.e. expressions of the structure $\langle a^\dagger a \ldots \rangle$. By an analogy to be explained then, objects of this type are generally called **correlation functions**. More important for our present discussion, at any finite temperature, the average $\langle \ldots \rangle$ entering the definition of the correlation function runs over the quantum Gibbs[7] distribution $\hat{\rho} \equiv e^{-\beta(\hat{H}-\mu\hat{N})}/\mathcal{Z}$, where, as usual,

$$\mathcal{Z} = \mathrm{tr}\; e^{-\beta(\hat{H}-\mu\hat{N})} = \sum_n \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle \,, \tag{4.23}$$

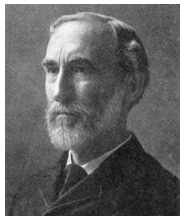
is the quantum partition function, $\beta \equiv 1/T$, μ denotes the chemical potential, and the sum extends over a complete set of Fock space states $\{|n\rangle\}$. (For the time being we neither specify the statistics of the system — bosonic or fermionic — nor the structure of the Hamiltonian.)

Ultimately, we will want to construct and evaluate the path integral representations of many–body correlation functions. Later we will see that all of these representations can be derived by a few straightforward manipulations form a prototypical path integral, namely that for $\mathcal{Z}$. Further, the (path integral of the) partition function is of importance in its own right: It contains much of the information needed to characterise the thermodynamic properties of a many–body quantum system.[8] We thus begin our journey into many–body field theory with a construction of the path integral for $\mathcal{Z}$.

To prepare the representation of the partition function (4.23) in terms of coherent states, one must insert the resolution of identity

$$\mathcal{Z} = \int d(\bar{\psi},\psi)\, e^{-\sum_i \bar{\psi}_i\psi_i} \sum_n \langle n|\psi\rangle\langle\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle \,. \tag{4.24}$$

We now wish to get rid of the — now redundant — Fock space summation over $|n\rangle$ (another resolution of identity). To bring the summation to the form $\sum_n |n\rangle\langle n| = \mathbf{1}_{\mathcal{F}}$,



Josiah Willard Gibbs 1839–1903: credited with the development of chemical thermodynamics, he introduced concepts of free energy and chemical potential.

[7]

[8] In fact, the statement above is not entirely correct. Strictly speaking thermodynamic properties involve the **thermodynamic potential** $\Omega = -T \ln \mathcal{Z}$ rather than the partition function itself. At first sight it seems that the difference between the two is artificial — one might first calculate $\mathcal{Z}$ and then take the logarithm. However, typically, one is unable to determine $\mathcal{Z}$ in closed form, but rather one has to perform a perturbative expansion, i.e. the result of a calculation of $\mathcal{Z}$ will take the form of a series in some small parameter ϵ. Now a problem arises when the logarithm of the series is taken. In particular, the Taylor series expansion of $\mathcal{Z}$ to a given order in ϵ does *not* automatically determine the expansion of Ω to the same order. Fortunately, the situation is not all that bad. It turns out that the logarithm essentially rearranges the combinatorial structure of the perturbation series in an order known as a **cumulant expansion**.

one must commute the factor $\langle n|\psi\rangle$ to the right hand side. However, in performing this seemingly innocuous operation, we must be careful not to miss a sign change whose presence will have important consequences for the structure of the fermionic path integral: Indeed, it may be checked that, whilst for bosons, $\langle n|\psi\rangle\langle\psi|n\rangle = \langle\psi|n\rangle\langle n|\psi\rangle$, the fermionic coherent states change sign upon permutation, $\langle n|\psi\rangle\langle\psi|n\rangle = \langle -\psi|n\rangle\langle n|\psi\rangle$ (i.e. $\langle -\psi| \equiv \exp\left(-\sum_i \bar{\psi}_i a_i\right)$). The presence of the sign is a direct consequence of the anti–commutation relations between Grassmann variables and Fock space operators (exercise). Note that, as both $\hat{H}$ and $\hat{N}$ contain elements even in the creation/annihilation operators, the sign is insensitive to the presence of the Boltzmann factor in (4.24). Making use of the sign factor ζ, the result of the interchange can be formulated as the general expression

$$\begin{aligned} \mathcal{Z} &= \int d(\bar{\psi},\psi)\, e^{-\sum_i \bar{\psi}_i\psi_i} \sum_n \langle\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle\langle n|\psi\rangle \\ &= \int d(\bar{\psi},\psi)\, e^{-\sum_i \bar{\psi}_i\psi_i} \langle\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle\,, \end{aligned} \tag{4.25}$$

where the equality is based on the identity $\sum_n |n\rangle\langle n| = \mathbf{1}_{\mathcal{F}}$. Eq. (4.25) can now be directly subjected to the general construction scheme of the path integral.

To be concrete, let us assume that the Hamiltonian is limited to a maximum of two–body interactions (cf. Eqs. (2.5) and (2.9)),

$$\hat{H}(a^\dagger,a) = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{ijkl} V_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l\,. \tag{4.26}$$

Note that, to facilitate the construction of the field integral, it is helpful to arrange for all of the annihilation operators to stand to the right of the creation operators. Fock space operators of this structure are said to be **normal ordered**.[9] The reason for emphasising normal ordering is that such an operator can be readily diagonalised by means of coherent states: Dividing the 'time interval' β into N segments and inserting coherent state resolutions of identity (steps 1, 2 and 3 of the general scheme), Eq. (4.25) assumes the form

$$\mathcal{Z} = \int_{\substack{\bar{\psi}^0=\zeta\bar{\psi}^N \\ \psi^0=\zeta\psi^N}} \prod_{n=0}^{N} d(\bar{\psi}^n,\psi^n)\, e^{-\delta\sum_{n=0}^{N-1}\left[\delta^{-1}(\bar{\psi}^n-\bar{\psi}^{n+1})\cdot\psi^n + H(\bar{\psi}^{n+1},\psi^n) - \mu N(\bar{\psi}^{n+1},\psi^n)\right]}\,, \tag{4.27}$$

where $\delta = \beta/N$ and $\frac{\langle\psi|\hat{H}(a^\dagger,a)|\psi'\rangle}{\langle\psi|\psi'\rangle} = \sum_{ij} h_{ij}\bar{\psi}_i\psi'_j + \sum_{ijkl} V_{ijkl}\,\bar{\psi}_i\bar{\psi}_j\psi'_k\psi'_l \equiv H(\bar{\psi},\psi')$, (similarly $N(\bar{\psi},\psi')$). Here, in writing Eq. (4.27), we have adopted the shorthand $\psi^n = \{\psi_i^n\}$, etc. Finally, sending $N\to\infty$ and taking limits analogous to those leading from (3.5) to

[9] More generally, an operator is defined to be 'normal ordered' with respect to a given vacuum state $|0\rangle$, if and only if, it annihilates $|0\rangle$. Note that the vacuum need not necessarily be defined as a zero particle state. If the vacuum contains particles, normal ordering need not lead to a representation where all annihilators stand to the right. If, for whatever reason, one is given a Hamiltonian whose structure differs from (4.26), one can always affect a normal ordered form at the expense of introducing commutator terms. For example, normal ordering the quartic term leads to the appearance of a quadratic contribution which can be absorbed into $h_{\alpha\beta}$.

(3.6) we obtain the continuum version of the path integral,[10]

$$\boxed{\mathcal{Z} = \int D(\bar{\psi},\psi) e^{-S[\bar{\psi},\psi]}, \qquad S[\bar{\psi},\psi] = \int_0^\beta d\tau \left[\bar{\psi}\partial_\tau \psi + H(\bar{\psi},\psi) - \mu N(\bar{\psi},\psi)\right]} \tag{4.28}$$

where $D(\bar{\psi},\psi) = \lim_{N\to\infty} \prod_{n=1}^N d(\bar{\psi}^n,\psi^n)$, and the fields satisfy the boundary condition

$$\bar{\psi}(0) = \zeta\bar{\psi}(\beta), \quad \psi(0) = \zeta\psi(\beta)\,. \tag{4.29}$$

Written in a more explicit form, the action associated with the general pair–interaction Hamiltonian (4.26) can be cast in the form

$$S = \int_0^\beta d\tau \left[\sum_{ij} \bar{\psi}_i(\tau)\left[(\partial_\tau - \mu)\delta_{ij} + h_{ij}\right]\psi_j(\tau) + \sum_{ijkl} V_{ijkl}\bar{\psi}_i(\tau)\bar{\psi}_j(\tau)\psi_k(\tau)\psi_l(\tau)\right]. \tag{4.30}$$

Notice that the structure of the action fits nicely into the general scheme discused in the previous chapter. By analogy, one would expect that the exponent of the many–body path integral carries the significance of the Hamiltonian action, $S \sim \int(p\dot{q} - H)$, where (q,p) symbolically stands for a set of generalized coordinates and momenta. In the present case, the natural pair of canonically conjugate operators is $(a, a^\dagger)$. One would then interpret the eigenvalues $(\psi,\bar{\psi})$ as 'coordinates' (much as (q,p) are the eigenvalues of the operators $(\hat{q},\hat{p})$). Adopting this interpretation, we see that the exponent of the path integral indeed has the canonical form of a Hamiltonian action and, therefore, is easy to memorize.

Eqs. (4.28) and (4.30) define the **functional integral in the time representation** (in the sense that the fields are functions of a time variable). In practice we shall mostly find it useful to represent the action in an alternative, Fourier conjugate representation. To this end, note that, due to the boundary conditions (4.29), the functions $\psi(\tau)$ can be interpreted as functions on the entire Euclidean time axis which are periodic/antiperiodic on the interval $[0,\beta]$. As such they can be represented in terms of a Fourier series,

$$\psi(\tau) = \frac{1}{\sqrt{\beta}}\sum_{\omega_n} \psi_n e^{-i\omega_n\tau}, \qquad \psi_n = \frac{1}{\sqrt{\beta}}\int_0^\beta d\tau\psi(\tau)e^{i\omega_n\tau}\,,$$

where

$$\omega_n = \begin{cases} 2n\pi T, & \text{bosons,} \\ (2n+1)\pi T, & \text{fermions} \end{cases}, \quad n\in\mathbb{Z} \tag{4.31}$$

are known as **Matsubara frequencies**. Substituting this representation into (4.28) and (4.30), we obtain $\mathcal{Z} = \int D(\bar{\psi},\psi)e^{-S[\bar{\psi},\psi]}$, where $D(\bar{\psi},\psi) = \prod_n d(\bar{\psi}_n,\psi_n)$ defines the

[10] Whereas the bosonic continuum limit is indeed perfectly equivalent to the one taken in constructing the quantum mechanical path integral ($\lim_{\delta\to 0}\delta^{-1}(\bar{\psi}^{n+1} - \bar{\psi}^n) = \partial_\tau|_{\tau=n\delta}$ gives an ordinary derivative etc.), a novelty arises in the fermionic case. The notion of replacing differences by derivatives is purely symbolic for Grassmann variables. There is no sense in which $\bar{\psi}^{n+1} - \bar{\psi}^n$ is small. The symbol $\partial_\tau\bar{\psi}$ rather denotes the formal (and well defined expression) $\lim_{\delta\to 0}\delta^{-1}(\bar{\psi}^{n+1} - \bar{\psi}^n)$.

measure (for each Matsubara index n we have an integration over a coherent state basis $\{|\psi_n\rangle\}$),[11] and the action takes the form

$$S[\bar{\psi},\psi] = \sum_{ij,\omega_n} \bar{\psi}_{in}\left[(-i\omega_n - \mu)\,\delta_{ij} + h_{ij}\right]\psi_{jn} + \frac{1}{\beta}\sum_{ijkl,\{\omega_{n_i}} V_{ijkl}\,\bar{\psi}_{in_1}\bar{\psi}_{jn_2}\psi_{kn_3}\psi_{ln_4}\delta_{n_1+n_2,n_3+n_4} \quad (4.32)$$

Here we have used the identity $\int_0^\tau d\tau e^{-i\omega_n\tau} = \beta\delta_{\omega_n,0}$. Eq. (4.32) defines the **frequency representation of the action**.[12]

▷ INFO. In performing calculations in the Matsubara representation, one sometimes runs into convergence problems (which will manifest themselves in the form of ill–convergent Matsubara frequency summations): In such cases it will be important to remember that Eq. (4.32) does not actually represent the precise form of the action. What is missing is a convergence generating factor whose presence follows from the way in which the integral was constructed, and which will save us in cases of non–convergent sums (except, of course, in cases where divergences have a physical origin). More precisely, since the fields $\bar{\psi}$ are evaluated infinitesimally later than the operators ψ (cf. Eq. (4.27)), the h and μ–dependent contributions to the action acquire a factor $\exp(-i\omega_n\delta)$, δ infinitesimal. Similarly, the V contribution acquires a factor $\exp(-i(\omega_{n_1}+\omega_{n_2})\delta)$. In cases where the convergence is not critical, we will omit these contributions. However, once in a while it is necessary to remember their presence.

4.2.1 Partition Function of Non–Interacting Gas

As a first exercise, let us consider the quantum partition function of the non–interacting gas. (Later, this object will prove useful as a 'reference' in the development of weakly interacting theories.) In some sense, the field integral formulation of the non–interacting partition function has a status similar to that of the path integral for the quantum harmonic osciallator: The direct quantum mechanical solution of the problem is straightforward and application of the full artillery of the field integral seems somewhat ludicrous. From a pedagogical point of view, however, the free partition function is a good problem; it provides us with the welcome opportunity to introduce a number of practical concepts of field integration within a comparatively simple setting. Moreover, the field integral representation of the free partition function will be an important operational building block for our subsequent analysis of interacting problems.

Consider, then the partition function (4.28) with $H_0(\bar{\psi},\psi) = \sum_{ij}\bar{\psi}_i H_{0,ij}\psi_j$. Diagonalising H_0 by a unitary transformation U, $H_0 = UDU^\dagger$ and transforming integration variables $U^\dagger\psi \equiv \phi$, the action assumes the form, $S = \sum_a\sum_{\omega_n}\bar{\phi}_{an}(-i\omega_n + \xi_a)\phi_{an}$, where $\xi_a \equiv \epsilon_a - \mu$ and ϵ_a are the single particle eigenvalues. Remembering that the fields $\phi_a(\tau)$

[11] Notice, however, that the fields ψ_n carry dimension $[\text{energy}]^{-1/2}$, i.e. the frequency coherent state integral is normalized as $\int d(\bar{\psi}_n,\psi_n)\,e^{-\bar{\psi}_n\epsilon\psi_n} = (\beta\epsilon)^{-\zeta}$.

[12] As for the signs of the Matsubara indices appearing in Eq. (4.32), note that the Fourier representation of $\bar{\psi}$ is defined as $\bar{\psi}(\tau) = \frac{1}{\sqrt{\beta}}\sum_n \bar{\psi}_n e^{+i\omega_n\tau}$, $\bar{\psi}_n = \frac{1}{\sqrt{\beta}}\int_0^\beta d\tau\,\bar{\psi}(\tau)e^{-i\omega_n\tau}$. In the bosonic case, this sign convention is motivated by $\bar{\psi}$ being the complex conjugate of ψ. For reasons of notational symmetry, this convention is also adopted in the fermionic case.

are independent integration variables (exercise: why does the transformation $\psi \to \phi$ have a Jacobian of unity?), we find that the partition function decouples, $\mathcal{Z} = \prod_a \mathcal{Z}_a$, where

$$\mathcal{Z}_a = \int D(\bar{\phi}_a, \phi_a)\, e^{-\sum_n \bar{\phi}_{an}(-i\omega_n+\xi_a)\phi_{an}} = \prod_n [\beta(-i\omega_n + \xi_a)]^{-\zeta}\,, \tag{4.33}$$

and the last equality follows from the fact that the integrals over ϕ_{an} are one–dimensional complex or Grassmann Gaussian integrals. Here, let us recall our convention defining $\zeta = 1(-1)$ for bosonic (fermionic) fields. At this stage, we have left all aspects of field integration behind us and reduced the problem to one of computing an infinite product over factors $i\omega_n - \xi_a$. Since products are usually more difficult to get under control than sums, we take the logarithm of $\mathcal{Z}$ to obtain the free energy

$$F = -T \ln \mathcal{Z} = -T\zeta \sum_{an} \ln[\beta(-i\omega_n + \xi_a)]\,. \tag{4.34}$$

▷ INFO. Before proceeding with this expression, let us take a second look at the intermediate identity (4.33). Our calcuation showed the partition function to be the product over all eigenvalues of the operator $-i\hat{\omega} + \hat{H} - \mu\hat{N}$ defining the action of the non-interacting system (here, $\hat{\omega} = \{\omega_n \delta_{nn'}\}$). As such, it can be written compactly as:

$$\boxed{\mathcal{Z} = \det\left[\beta(-i\hat{\omega} + \hat{H} - \mu\hat{N})\right]^{-\zeta}} \tag{4.35}$$

This result was derived by first converting to an eigenvalue integration and then performing the one–dimensional integrals over 'eigencomponents' ϕ_{an}. While technically straightforward, that — explicitly representation-dependent — procedure is not well suited to generalization to more complex problems. (Keep in mind that later on we will want to embed the free action of the non–interacting problem into the more general framework of an interacting theory.)

Indeed, it is not necessary to refer to an eigenbasis at all: In the bosonic case, Eq. (3.17) tells us that Gaussian integration over a bilinear $\sim \bar{\phi}\hat{X}\phi$ generates the inverse determinant of $\hat{X}$. Similarly, as we have seen, Gaussian integration extends to the Grassmann case with the determinants appearing in the numerator rather than in the denominator (as exemplified by (4.35)). (As a matter of fact, (4.33) is already a proof of this relation.)

We now have to face up to a technical problem: How do we compute Matsubara sums of the form $\sum_n \ln(i\omega_n - x)$? Indeed, it takes little imagination to foresee that sums of the type $\sum_{n_1,n_2,\ldots} X(\omega_{n_1}, \omega_{n_2}, \ldots)$, where X symbolically stands for some function, will be a recurrent structure in the analysis of functional integrals. A good ansatz would be to argue that, for sufficiently low temperatures (i.e. temperatures smaller than any other characteristic energy scale in the problem), the sum can be traded for an integral, viz. $T\sum_n \to \int d\omega/(2\pi)$. However, this approximation is too crude to capture much of the characteristic temperature dependence in which one is usually interested. Yet there exists an alternative, and much more accurate way of computing sums over Matsubara frequencies:

▷ INFO. Consider a single **Matsubara frequency summation**,

$$S \equiv \sum_n h(\omega_n)\,, \tag{4.36}$$

where h is some function and ω_n may be either bosonic or fermionic (cf. Eq. (4.31)). The basic idea behind the standard scheme of evaluating sums of this type is to introduce a complex auxiliary function $g(z)$ that has simple poles at $z = i\omega_n$. The sum S then emerges as the sum of residues obtained by integrating the product gh along a suitably chosen path in the complex plane. Typical choices of g include

$$g(z) = \begin{cases} \dfrac{\beta}{\exp(\beta z) - 1}, & \text{bosons} \\ \dfrac{\beta}{\exp(\beta z) + 1}, & \text{fermions} \end{cases} \quad \text{and} \quad g(z) = \begin{cases} \dfrac{\beta}{2}\coth(\beta z/2), & \text{bosons} \\ \dfrac{\beta}{2}\tanh(\beta z/2), & \text{fermions} \end{cases} \tag{4.37}$$

where, in much of this section, we will employ the functions of the first column. (Notice the similarity between these functions and the familiar Fermi and Bose distribution functions.) In practice, the choice of the counting function is mostly a matter of taste, save for some cases where one of the two options is dictated by convergence criteria.

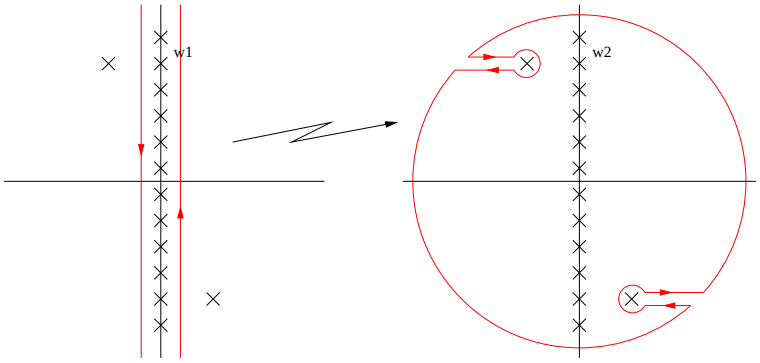


Figure 4.2: Left: the integration contour employed in calculating the sum (4.36). Right: the deformed integration contour.

Integration over the path shown in the left part of Fig. 4.2 then produces

$$\frac{\zeta}{2\pi i}\oint dz g(z)h(-iz) = \zeta\sum_n \mathrm{Res}\,(g(z)h(-iz))|_{z=i\omega_n} = \sum_n h(\omega_n) = S\,,$$

where, in the third identity, we have used the fact that the 'counting functions' g are chosen so as to have residue ζ and it is assumed that the integration contour closes at $z \to \pm i\infty$. (The difference between using the first and the second column of (4.37) lies in the value of the residue. In the latter case, it is equal to unity rather than ζ.) Now, the integral along a contour in the immediate vicinity of the poles of g is usually intractable. However, as long as we are careful not to cross any singularities of g or the function $h(-iz)$ (the latter symbolically indicated by isolated crosses in the figure[13]) we are free to distort the integration path, ideally to a contour along

[13]Remember that a function that is bounded and analytic in the entire complex plane is constant, i.e. every 'interesting' function will have singularities.

which the integral *can* be performed. Finding a suitable contour is not always straightforward. If the product hg decays sufficiently fast at $|z| \to \infty$ (i.e. faster than z^{-1}), one will ususally try to 'inflate' the original contour to an infinitely large circle (Fig. 4.2, right).[14] The integral along the outer perimeter of the contour then vanishes and one is left with the integral around the singularities of the function h. In the simple case where $h(-iz)$ posesses a number of isolated singularities at $\{z_k\}$ (i.e. the situation indicated in the figure) we thus obtain[15]

$$S = -\frac{\zeta}{2\pi i}\oint h(-iz)g(z) = -\zeta\sum_k \operatorname{Res} h(-iz)g(z)|_{z=z_k}\,, \tag{4.38}$$

i.e. the task of computing the infinite sum S has been reduced to that of evaluating a finite number of residues — a task that is always possible!

To illustrate the procedure on a simple example, let us consider the function

$$h(\omega_n) = -\frac{\zeta T}{i\omega_n e^{-i\omega_n\delta} - \xi}\,,$$

where δ is a positive infinitesimal.[16] To evaluate the sum $S = \sum_n h(\omega_n)$, we first observe that the product $h(-iz)g(z)$ has benign convergence properties. Further, the function $h(-iz)$ has a simple pole that, in the limit $\delta \to 0$, lies on the real axis at $z = \xi$. This leads to the result

$$\sum_n h(\omega_n) = \zeta \operatorname{Res} g(z)h(-iz)|_{z=\xi} = -\frac{1}{e^{\beta\xi} - \zeta}\,.$$

We have thus arrived at the important identity

$$\boxed{\zeta T\sum_n \frac{1}{i\omega_n - \xi_a} = \begin{cases} n_{\rm B}(\epsilon_a), & \text{bosons,} \\ n_{\rm F}(\epsilon_a), & \text{fermions} \end{cases}} \tag{4.39}$$

[14]Notice that the condition $\lim_{|z|\to\infty}|hg| < z^{-1}$ is not as restrictive as it may seem. The reason is that the function h will be mostly related to physical observables that approach some limit (or vanish) for large excitation energies. This implies vanishing in at least portions of the complex plane. The convergence properties of g depend on the concrete choice of the counting function. (Exercise: explore the convergence properties of the functions shown in Eq. (4.37).)

[15]If you are confused about signs, note that the contour encircles the singularities of h in a clockwise direction.

[16]Indeed, this choice of h is actually not as artificial as it may seem. The expectation value of the **number of particles** in the grand canonical ensemble is defined through the identity $N \equiv -\partial F/\partial\mu$ where F is the free energy. In the non–interacting case, the latter is given by Eq. (4.34) and, remembering that $\xi_a = \epsilon_a - \mu$, one obtains $N \approx -\zeta T\sum_{an}\frac{1}{i\omega_n - \xi_a}$. Now, why did we write '$\approx$' instead of '$=$'? The reason is that the right hand side, obtained by naive differentiation of (4.34), is ill–convergent. (The sum $\sum_{n=-\infty}^{\infty}\frac{1}{n+x}$, x arbitrary, does not exist!) At this point we have to remember the remark made in the on page 136, i.e., had we carefully treated the discretisation of the field integral, both the logarithm of the free energy and $\partial_\mu F$ would acquire infinitesimal phases $\exp(-i\omega_n\delta)$. As an exercise, try to keep track of the discretisation of the field integral from its definition to Eq. (4.34) to show that the accurate expression for N reads

$$N = -\zeta T\sum_{an}\frac{1}{i\omega_n e^{-i\omega_n\delta} - \xi_a} = \sum_a\sum_n h(\omega_n)\big|_{\xi=\xi_a}\,,$$

where h is the function introduced above. (Note that the necessity to keep track of the lifebuoy $e^{-i\omega_n\delta}$ does not arise too often. Most Matsubara sums of physical interest relate to functions f that decay faster than z^{-1}.)

where

$$n_{\rm F}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1}, \qquad n_{\rm B}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}-1} \tag{4.40}$$

are the Fermi/Bose distribution functions. As a corollary we note that the expectation value for the number of particles in a non–interacting quantum gas assumes the familiar form $N = \sum_a n_{\rm F/B}(\epsilon_a)$.

Before returning to our discussion of the partition function, let us note that life is not always as simple as the example above. More often than not, the function h not only contains isolated singularities but also cuts or worse singularities. Under such circumstances, finding a good choice of the integration contour can be far from straightforward!

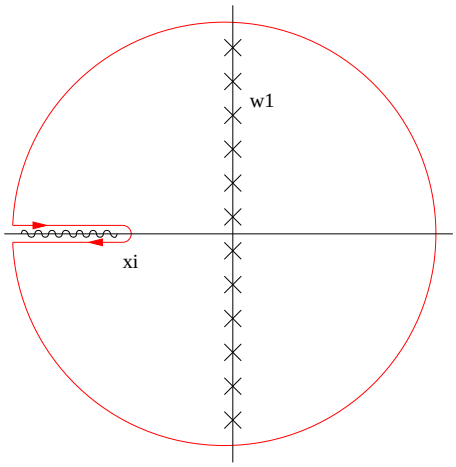


Figure 4.3:

Returning to the problem of computing the sum (4.34), consider for a moment a fixed eigenvalue $\xi_a \equiv a$. In this case, we need to evaluate the sum $S \equiv \sum_n h(\omega_n)$, where $h(\omega_n) \equiv \zeta T \ln[\beta(-i\omega_n + \xi)] = \zeta T \ln[\beta(i\omega_n - \xi)] + C$ and C is an inessential constant. As discussed before, the sum can be represented as $S = -\frac{\zeta}{2\pi i}\oint g(z)h(-iz)$, where $g(z) = \beta(e^{\beta z} - \zeta)^{-1}$ is (β times) the distribution function and the contour encircles the poles of g as in Fig. 4.2, left. Now, there is an essential difference with the example discussed previously, viz. the function $h(-iz) = \zeta T \ln(z - \xi) + C$ has a branch cut along the real axis, $z \in (-\infty, \xi)$ (see the figure). To avoid contact with this singularity one must distort the integration contour as shown in the figure. Noticing that the (suitably regularized, cf. our previous discussion of the particle number N) integral along the perimeter vanishes, we conclude that

$$S = \frac{T}{2\pi i}\int_{-\infty}^{\infty} d\epsilon\, g(\epsilon)\left(\ln(\epsilon^+ - \xi) - \ln(\epsilon^- - \xi)\right) ,$$

where $\epsilon^{\pm} = \epsilon \pm i\eta$, η is a positive infinitesimal, and we have used the fact that $g(\epsilon^{\pm}) \simeq g(\epsilon)$ is continuous across the cut. (Also, without changing the value of the integral (exercise: why?), we have enlarged the integration interval from $(-\infty, \xi]$ to $(-\infty, \infty)$). To evaluate

the integral, we observe that $g(\epsilon) = -\zeta\partial_\epsilon \ln\left(1-\zeta e^{-\beta\epsilon}\right)$ and integrate by parts:

$$S = -\frac{\zeta T}{2\pi i}\int d\epsilon\, \ln\left(1-\zeta e^{-\beta\epsilon}\right)\left(\frac{1}{\epsilon^+-\xi}-\frac{1}{\epsilon^--\xi}\right) \stackrel{(3.58)}{=} \zeta T \ln\left(1-\zeta e^{-\beta\xi}\right) .$$

Insertion of this result into Eq. (4.34) finally obtains the familiar expression

$$F = \zeta T \sum_a \ln\left(1-\zeta e^{-\beta(\epsilon_a-\mu)}\right) \tag{4.41}$$

for the free energy of the non–interacting Fermi/Bose gas. While this result could have been obtained much more straightforwardly by the methods of quantum statistical mechanics, we will shortly see how powerful a tool the methods discussed in this section are when it comes to the analysis of less elementary problems!

4.3 Summary and Outlook

This concludes our preliminary introduction to the field integral. We have learned how to represent the partition function of a quantum many–body system in terms of a generalized path integral. The field integral representation of the partition function will be the basic platform on which all our further developments will be based. In fact, we are now in a position to face up to the main problem addressed in this text: practically none of the 'non–trivial' field integrals in which one might be interested can be executed in closed form. This reflects the fact that, save for a few exceptions, interacting many–body problems do not admit closed solutions. In the following chapter, we will introduce approximation stratgies for addressing interacting theories by exploring some physical applications of the field integral.

Chapter 5

Broken Symmetry and Collective Phenomena

Previously, we have seen how the field integral method can be deployed in many-particle theories. In the following chapter, we will learn how elements of perturbation theory can be formulated efficiently by staying firmly within the framework of the field integral. In doing so, we will see how the field integral provides a method for identifying and exploring non-trivial reference ground states — 'mean–fields'. A fusion of perturbative and mean–field methods will provide us with analytical machinery powerful enough to address a spectrum of rich applications.

Historically, the effects of interaction on many-body systems are typically dealt with within the framework of "diagrammatic" perturbation theory, a series expansion in the interaction strength. However, in the following, we will search for a different methodology. Our motivations are two-fold: Firstly, the structures that typically appear from perturbative expansions can be assimilated more straightforwardly. But, more importantly, the development of phase instabilities typically reflect the appearance of non-perturbative structures. Thus, what we would like to develop is a theoretical framework that is capable of (a) detecting the 'right' reference states or 'mean-fields' of a system, (b) that enables us to efficiently apply perturbative methods around these states and, finally, (c) to do this in a language that draws upon the 'physical' rather than the plain microscopic degrees of freedom as the fundamental units.

To this end, in the following sections we will develop a functional integral based approach that meets these criteria. In contrast to the previous chapters, the discussion here will be decidedly biased towards concrete application to physically motivated problems. After the formulation of the general strategy of field integral based mean-field methods, the next section will address the problem of the weakly interacting electron gas. The exemplification of the new concepts on "familiar territory" will enable us to better understand the intimate connection between the mean-field approach and straightforward perturbation theory. In subsequent sections we will then turn to the discussion of problems which lie firmly outside the range of direct perturbative summation, viz. the phenomena of superfluidity and superconductivity.

5.1 Mean-Field Theory

Roughly speaking, the functional approach to problems with a large parameter proceeds according to the following programme:

1. In the first place, one must identify the relevant structural units of the theory. (This part of the programme *can* be efficiently carried out by the straightforward methods discussed earlier.)

2. Secondly, it is necessary to introduce a new field — let us call it ϕ for concreteness — that encapsulates the relevant degrees of freedom of the low energy theory.

3. With this in hand, one can then trade integration over the 'microscopic fields' for an integration over ϕ, a step often effected by an operation known as the Hubbard–Stratonovich transformation.

4. The low–energy content of the theory can often be explored by subjecting the resulting action $S[\phi]$ to a stationary phase analysis. (The justification for applying stationary phase methods is provided by the existence of a large parameter $N \gg 1$.) Often, at this stage, instabilities in the theory show up — an indication of a physically interesting problem!

5. Finally, the nature of the elementary (collective) excitations above the ground state can by explored by expanding the functional integral around the solution of the stationary phase equations — the 'mean-field'. From this low-energy effective action, one can compute physical observables.

In the next section, we will illustrate how such a programme can be implemented on a specific example which can also be studied by perturbative means:

5.2 Plasma Theory of the Interacting Electron Gas

In first quantised form, the *weakly* interacting electron gas is described by the many-body Hamiltonian,

$$\boxed{\hat{H} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}} \tag{5.1}$$

For simplicity, we have chosen to neglect to presence of any underlying lattice potential. Formally, the corresponding quantum partition function is obtained as $\mathcal{Z} = \mathrm{tr} e^{-\beta(\hat{H}-\mu\hat{N})}$ where the trace runs over a complete basis of many-body states.

▷ Info. Before plunging into the computation of the quantum partition function from the coherent state path integral we should first try to understand in what limit Coulomb interactions may be thought of as *weak*. In fact, the control parameter is the average density of the electron gas: $n \equiv 1/r_0^3$ where r_0 denotes the average interelectron spacing. Coulomb interaction is weak

when the average potential energy (measured in units of e^2/r_0) is small as compared to the typical kinetic energy (measured in units of $\hbar^2/mr_0^2$). The ratio of energy scales defines the **dimensionless density parameter**

$$\frac{e^2}{r_0}\frac{mr_0^2}{\hbar} = \frac{r_0}{a_0} \equiv r_s,$$

where $a_0 = \hbar/e^2m$ denotes the Bohr radius. Physically, r_s is the radius of the spherical volume containing one electron on average; the denser the electron gas, the smaller r_s.

Below, we will be concerned with the limit of high density $r_s \ll 1$, in which the effects of Coulomb interaction can be treated perturbatively. In the opposite limit, $r_s \gg 1$, properties become increasingly dominated by the Coulomb interaction. Ultimately, for sufficiently large r_s (or low density) it is believed that the electron gas undergoes a (first order) phase transition to a condensed or 'solid' phase known as a **Wigner crystal**. (Indeed, this phenomenon is the continuum counterpart of the Mott-Hubbard transition described in section 2.2.3.) Although Wigner[1] crystals have never been unambiguously observed, several experiments performed on low density electron gases are consistent with a Wigner crystal ground state. Quantum Monte-Carlo simulation suggests that Wigner crystallisation may occur for densities $r_s > 37$. (Note that this scenario relies crucially on being at low temperatures, and the long-range nature of the Coulomb interaction. In particular, if the Coulomb interaction is screened $V(r) \sim e^{-r/\lambda}$, $r_s \sim (r_0/a_0)e^{-r_0/\lambda}$ and the influence of Coulomb interaction at high densities becomes diminished.)

For $r_s \sim O(1)$, the potential and kinetic energies are comparable. This regime of intermediate coupling is notoriously difficult to describe quantitatively. Yet most metals lie in a regime of intermediate coupling $2 < r_s < 6$. Fortunately, there is overwhelming evidence to suggest that a *weak coupling* description holds even well outside the regime over which microscopic theory can be justified. The phenomenology of the intermediate coupling regime is the realm of **Landau's Fermi Liquid Theory**.

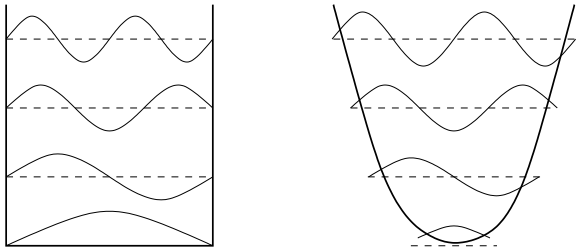


Figure 5.1: Sketch showing the adiabatic continuity of the eigenstates in a one-dimensional potential well.

The fundamental principle underlying the Fermi liquid theory is one of "adiabatic continuity" [5]: In the absence of an electronic phase transition (such as Wigner crystallisation or

Eugene P. Wigner 1902-1995; 1963 Nobel Laureate in Physics for his contributions to the theory of the atomic nucleus and the elementary particles, particularly through the discovery and application of fundamental symmetry [1]principles.

the Mott transition), a non-interacting ground state evolves smoothly or adiabatically into the interacting ground state as the strength of interaction is increased.[2] An elementary excitation of the non-interacting system represents an "approximate excitation" of the interacting system (i.e. the 'lifetime' of an elementary excitation is long). Excitations are quasi-particles (and quasi-holes) above a sharply defined Fermi surface. The remarkable success (as well as the few notorious failures) of Landau Fermi liquid theory[3] make the subject an important area of modern condensed matter physics but one which we will not have time to explore. Instead, motivated in part by the success of Fermi liquid theory, we will proceed to explore the quantum partition function of the *weakly* interacting electron gas, $r_s \ll 1$.

To prepare for a discussion of the field integral, we must first recast the Hamiltonian in second quantised form as

$$\hat{H} = \int d^3r c_\sigma^\dagger \frac{\hat{\mathbf{p}}^2}{2m} c_\sigma + \frac{1}{2}\int d^3r\, d^3r' c_\sigma^\dagger(\mathbf{r}) c_{\sigma'}^\dagger(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} c_{\sigma'}(\mathbf{r}') c_\sigma(\mathbf{r}),$$

where the sum over repeated spin indicies σ is here implied. When cast as functional field integral, the corresponding quantum partition function takes the form $\mathcal{Z} \equiv \mathrm{tr}(e^{-\beta(\hat{H}-\mu\hat{N})}) = \int D(\bar{\psi},\psi) e^{-S}$, where

$$S[\psi,\bar{\psi}] = \int_0^\beta d\tau \int d^3r \bar{\psi}_\sigma \left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu\right)\psi_\sigma + \frac{1}{2}\int_0^\beta d\tau \int d^3r\, d^3r'\, \bar{\psi}_\sigma(\mathbf{r})\bar{\psi}_{\sigma'}(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}),$$

Employing the "four-vector" shorthand $x = (\tau, \mathbf{r})$ and $q = (\omega_m, \mathbf{q})$, where ω_m denotes a bosonic Matsubara frequency (exercise: think why), we may define the "density field" $\rho_q = \frac{1}{\sqrt{\beta}}\int dx e^{iq\cdot x}\bar{\psi}_\sigma(x)\psi_\sigma(x) = \frac{1}{\sqrt{\beta}}\sum_p \bar{\psi}_{p\sigma}\psi_{p+q\sigma}$ (with $\int dx \equiv \int_0^\beta d\tau \int d^3r$ and $q\cdot x \equiv \omega_m\tau - \mathbf{q}\cdot\mathbf{r}$). Then, expressed in the Fourier basis, the action takes the form (exercise)

$$S[\psi,\bar{\psi}] = \sum_p \bar{\psi}_{p\sigma}\left(-i\omega_n + \frac{\mathbf{p}^2}{2m} - \mu\right)\psi_{p\sigma} + \frac{1}{2L^3}{\sum_q}' \rho_q V(\mathbf{q}) \rho_{-q},$$

[2] As a simple non-interacting example, consider the adiabatic evolution of the bound states of a quantum particle as the confining potential is changed from a box to a harmonic potential well (see Fig. 5.1). While the wavefunctions and energies evolve, the topological characteristics of the wavefunctions, i.e. the number of the nodes, and therefore the assignment of the corresponding quantum numbers remains unchanged.

[3] L. D. Landau, Sov. Phys. JETP **3**, 920 (1956); *ibid.* **5**, 101 (1957).

Lev D. Landau 1908-1968, 1962 Nobel Laureate in Physics for his pioneering theories for condensed matter, especially liquid helium.

where $V(\mathbf{q}) = \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{r}) = 4\pi e^2/\mathbf{q}^2$.[4] Here, the prime on the q summation denotes the exclusion of the $\mathbf{q} = 0$ contribution and reflects the presence of a neutralising background charge.

Now, being quartic in the fields ψ_σ, the Coulomb interaction prevents an explicit computation of the functional ψ–integral. However, it is actually a straightforward matter to reduce, or 'decouple' the interaction operator bringing it to a form quadratic in the fields ψ. Let us multiply the functional integral by the 'fat unity'

$$1 \equiv \mathcal{N} \int D\phi \, \exp\left[-\frac{e^2}{2} \sum_q \phi_q V^{-1}(\mathbf{q}) \phi_{-q} \right] ,$$

where ϕ represents a complex bosonic field variable, and a normalization constant has been absorbed in the definition of the functional measuere $D\phi$. Employing the variable shift $e\phi_q \mapsto e\phi_q + \frac{i}{L^{3/2}} V(\mathbf{q})\rho_q$, one obtains

$$1 = \int D\phi \, \exp\left[\sum_q \left(-\frac{e^2}{2} \phi_q V^{-1}(\mathbf{q}) \phi_{-q} - \frac{i}{L^{3/2}} e\rho_q \phi_{-q} + \frac{1}{2L^3} \rho_q V(\mathbf{q}) \rho_{-q} \right) \right] .$$

The rational behind this exercise can be seen in the last contribution to the exponent: This term is equivalent to the quartic interaction contribution to the fermionic path integral, albeit with opposite sign. Therefore, multiplication of $\mathcal{Z}$ by our unity leads to the field integral $\mathcal{Z} = \int D\phi \int D(\bar\psi_\sigma, \psi_\sigma) e^{-S}$, where

$$S = \frac{1}{8\pi} \sum_q \phi_q \mathbf{q}^2 \phi_{-q} + \sum_{pp'} \bar\psi_{p\sigma} \left[\left(-i\omega_n + \frac{\mathbf{p}^2}{2m} - \mu \right) \delta_{pp'} + \frac{i}{\sqrt{\beta L^3}} e\phi(p'-p) \right] \psi_{p'\sigma} \, , \quad (5.2)$$

denotes the action, i.e. an expression that is free of quartic field interactions of ψ_σ. Before proceeding, to acquire some intuition for the nature of the action, it is helpful to rewrite S in a real space/time representation. With $\phi_q = \frac{1}{\sqrt{\beta L^3}} \int dx \, e^{-iq\cdot x} \phi(x)$ (four-vector notation as above), one may confirm that,

$$S[\phi, \bar\psi, \psi] = \int_0^\beta d\tau \int d^3r \left\{ \frac{1}{8\pi} (\partial\phi)^2 + \bar\psi_\sigma \left[\partial_\tau - \frac{\partial^2}{2m} - \mu + ie\phi \right] \psi_\sigma \right\} .$$

Physically, ϕ couples to the electron degrees of freedom as a space/time dependent (imaginary) scaler potential, while the first term reflects the Lagrangian energy density associated with the electric component of the electromagnetic (alias the photon) field. Said differently, the field ϕ represents the gauge particle — in this case, the photon — that mediates the Coulomb interaction between electrons. Before proceeding, let us now step back and discuss the general philosophy of the manipulations that led from the original partition function to the two-field representation (5.2).

▷ INFO. The sequence of manipulations developed above, i.e. the 'decoupling' of a quartic interaction through an auxiliary field, is known more generally as a **Hubbard–Stratonovich**

[4] By representing Poisson's equation for a point charge in the Fourier space, one may confirm that $\frac{1}{L^3} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{q}) = \frac{e^2}{|\mathbf{r}|}$.

transformation. The essence of the transformation is a straightforward manipulation of a Gaussian integral. To make this point more transparent, let us reformulate the Hubbard-Stratonovich transformation in a notation that is not burdened by the presence of model–specific constants. Consider an interaction operator of the form $S_{\rm int} = V_{\alpha\beta\gamma\delta}\,\bar\psi_\alpha\psi_\beta\bar\psi_\gamma\psi_\delta$ (summation convention implied), where $\bar\psi$ and ψ may be either bosonic or fermionic field variables, the indices $\alpha, \beta, \ldots$ refer to an unspecified set of quantum numbers, Matsubara frequencies, etc., and $V_{\alpha\beta\gamma\delta}$ is an interaction matrix element. Now, let us introduce composite operators $\hat\rho_{\alpha\beta} \equiv \bar\psi_\alpha\psi_\beta$ to rewrite the interaction as $S_{\rm int} = V_{\alpha\beta\gamma\delta}\,\hat\rho_{\alpha\beta}\hat\rho_{\gamma\delta}$. The notation can be compactified still further by introducing composite indices $m \equiv (\alpha\beta)$, $n \equiv (\gamma\delta)$, whereupon the action $S_{\rm int} = \hat\rho_m V_{mn}\hat\rho_n$ acquires the structure of a generalized bilinear form. To reduce the action to a form quadratic in the ψs one may simply multiply the exponentiated action by unity, viz.

$$e^{-\hat\rho_m V_{mn}\hat\rho_n} = \underbrace{\int D\phi\, e^{-\frac{1}{4}\phi_m V^{-1}_{mn}\phi_n}}_{1}\, e^{-\hat\rho_m V_{mn}\hat\rho_n}\,,$$

where ϕ is bosonic. (Notice that here V^{-1}_{mn} represents the matrix elements of the inverse and not the inverse $(V_{mn})^{-1}$ of individual matrix elements.) Finally, applying the variable change $\phi_m \to \phi_m + 2i(V\hat\rho)_m$ where the notation $(V\hat\rho)$ is shorthand for $V_{mn}\hat\rho_n$, one obtains

$$\boxed{\exp\left[-\hat\rho_m V_{mn}\hat\rho_n\right] = \int D\phi\, \exp\left[-\frac{1}{4}\phi_m V^{-1}_{mn}\phi_n - i\phi_m\hat\rho_n\right]}$$

I.e. the term quadratic in $\hat\rho$ is cancelled.[5] This completes the formulation of the Hubbard-Stratonovich transformation. The interaction operator has been traded for (a) an integration over an auxiliary field coupled (b) to a ψ-bilinear (the operator $\phi_m\hat\rho_m$).

- ▷ In essence, the Hubbard-Stratonovich transformation is tantamount to Gaussian integral identity (3.13) but read in reverse. An exponentiated square is removed in exchange for a linear coupling. (In (3.13) we showed how terms linear in the integration variable can be removed.)

- ▷ To make the skeleton outlined above a well defined prescription, one has to be more specific about the meaning of the Gaussian integration over the kernel $\phi_m V^{-1}_{mn}\phi_n$, i.e. the integration variables can be real or complex, and V must be a positive matrix (which is usually the physical situation).

- ▷ There is some freedom as to the choice of the integration variable. For example, the factor of 1/4 in front of the Gaussan weight $\phi_m V^{-1}_{mn}\phi_n$ was introduced for mere convenience (viz. to generate a coupling $\phi_m\hat\rho_m$ free of numerical factors). If one does not like to invert the matrix kernel V_{mn}, one can scale $\phi_m \to (V\phi)_m$, whereupon the key formula reads

$$e^{-\hat\rho_m V_{mn}\hat\rho_n} = \int D\phi\, e^{-\frac{1}{4}\phi_m V_{mn}\phi_n - i\phi_m V_{mn}\hat\rho_n}\,.$$

▷ Exercise. Show that the passage from the Lagrangian to the Hamiltonian formulation of the Feynman path integral can be interpreted as a Hubbard–Stratonovich transformation.

[5] Here we have assumed that the matrix V is symmetric. If it is not, we can apply the relation $\hat\rho_m V_{mn}\hat\rho_n \equiv \hat\rho^T V\hat\rho = \frac{1}{2}\left[\hat\rho^T(V + V^T)\hat\rho\right]$ to symmetrize the interaction.

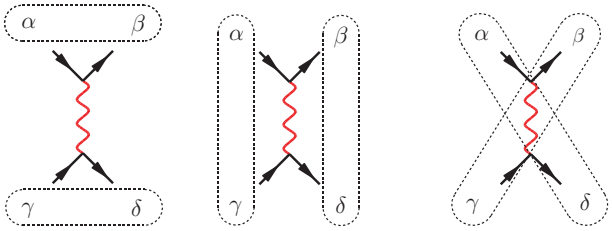


Figure 5.2: On the different channels of decoupling an interaction by Hubbard-Stratonovich transformation. Left: decoupling in the 'density' channel; middle: decoupling in the 'pairing' or 'Cooper' channel; and right: decoupling in the 'exchange' channel.

As defined, the Hubbard-Stratonovich transformation is exact. However, to make it a meaningful operation, it must be motivated by some physical considerations. In our discussion above, we split up the interaction by choosing $\hat{\rho}_{\alpha\beta}$ as a composite operator. However, there is clearly some arbitrariness with this choice. Why not, for example, pair the fermion–bilinears according to $(\bar{\psi}_\alpha\psi_\delta)(\bar{\psi}_\gamma\psi_\delta)$, or otherwise? The three inequivalent choices of pairing up operators are shown in Fig. 5.2 where, as usual, the wavy line with attached field vertices represents the interaction, and the dashed ovals indicate how the field operators are paired.

The version of the transformation discussed above corresponds to the left diagram of the figure. That type of pairing is sometimes referred to as decoupling in the **direct channel**. The denotation becomes more transparent if we consider the example of the spinfull electron-electron interaction,

$$S_{\rm int} = \frac{1}{2}\int d\tau \int d^3r\, d^3r'\, \bar{\psi}_\sigma(\mathbf{r},\tau)\bar{\psi}_{\sigma'}(\mathbf{r}',\tau)V(\mathbf{r}-\mathbf{r}')\psi_{\sigma'}(\mathbf{r}',\tau)\psi_\sigma(\mathbf{r},\tau),$$

i.e. here $\alpha=\beta=(\mathbf{r},\tau,\sigma)$, $\gamma=\delta=(\mathbf{r}',\tau,\sigma')$, and $V_{\alpha\beta\gamma\delta}=V(\mathbf{r}-\mathbf{r}')$. The 'direct' decoupling proceeds via the most obvious choice, i.e. the density operator $\hat{\rho}(\mathbf{r},\tau)=\bar{\psi}_\sigma(\mathbf{r},\tau)\psi_\sigma(\mathbf{r},\tau)$. One speeks about decoupling in a 'channel' because, as will be elucidated below, the propagator of the decoupling field can be interpreted in terms of two Green function lines tied together by multiple interactions, a sequential object reminiscent of a 'channel'.

However, more important than the terminology is the fact that there are other choices for ρ. Decoupling in the **exchange channel** is generated by the choice $\rho_{\alpha\gamma}\sim\bar{\psi}_\alpha\psi_\delta$ where, in the context of the Coulomb interaction, the reversed pairing of field operators is reminiscent of the exchange contraction generating Fock–type contributions. Finally, one may decouple in the **Cooper channel**, $\hat{\rho}=\bar{\psi}_\alpha\bar{\psi}_\gamma$, $\rho_{\beta\gamma}=\rho^\dagger_{\gamma\beta}$. Here, the pairing field is conjugate to two creation operators. Below we will see that this type of decoupling is tailored to problems involving superconductivity.

The remarks above may convey the impression of a certain arbitrariness inherent in the Hubbard-Stratonovich scheme. Indeed, the 'correct' choice of decoupling can only be motivated by physical reasoning, not by plain mathematics. Put differently, the transformation as such is exact, no matter what channel we choose. However, later, we will want to derive an effective low energy theory based on the decoupling field. In cases where one has accidentally decoupled in an 'unphysical' channel, it will be difficult, if not impossible to distill a meaningful low energy theory for the field ϕ conjugate to ρ. Although the initial model still contains the full microscopic information (by virtue of the exactness of the transformation) it is not amenable to further approximation schemes.

In fact, one is frequently confronted with situations where more than one Hubbard-Stratonovich field is needed to capture the full physics of the problem. To appreciate this point, consider the

Coulomb interaction in momentum space.

$$S_{\rm int}[\bar\psi,\psi] = \frac{1}{2}\sum_{p_1,\ldots,p_4} \bar\psi_{\sigma p_1}\bar\psi_{\sigma' p_3} V(\mathbf{p}_1-\mathbf{p}_2)\psi_{\sigma' p_4}\psi_{\sigma p_2}\,\delta_{p_1-p_2+p_3-p_4}\,. \tag{5.3}$$

In principle, we can decouple this interaction in any one of the three channels discussed above. However, 'interesting' physics is usually generated by processes where one of the three unbound momenta entering the interaction vertex is small. Only these interaction processes have a chance to accumulate an overall collective excitation of low energy (cf. many of the examples to follow). It may be instructive to imagine the situation geometrically: In the three dimensional cartesian space of free momentum coordinates (p_1,p_2,p_3) entering the vertex, there are three thin layers where one of the momenta is small, (q,p_2,p_3), (p_1,q,p_3), (p_1,p_2,q), $|q|\ll|p_i|$. (Why not make all momenta small? Because that would be in conflict with the condition that the Green functions connecting to the vertex be close to the Fermi surface.) One will thus often choose to break down the full momentum summation to a restricted summation over the small–momentum sublayers:

$$S_{\rm int}[\bar\psi,\psi] \simeq \frac{1}{2}\sum_{p,p',q}\Big(\bar\psi_{\sigma p}\psi_{\sigma p+q}V(\mathbf{q})\bar\psi_{\sigma' p'}\psi_{\sigma' p'-q} - \bar\psi_{\sigma p}\psi_{\sigma' p+q}V(\mathbf{p}'-\mathbf{p})\bar\psi_{\sigma' p'+q}\psi_{\sigma p'} - \bar\psi_{\sigma p}\bar\psi_{\sigma' -p+q}V(\mathbf{p}'-\mathbf{p})\psi_{\sigma p'}\psi_{\sigma' -p'+q}\Big)\,.$$

Now, each of these three contributions has its own predestined choice of a slow decoupling field. The first term should be decoupled in the direct channel $\hat\rho_{{\rm d},q}\sim\sum_p\bar\psi_{\sigma p}\psi_{\sigma p+q}$, the second in the exchange channel $\hat\rho_{{\rm x},\sigma\sigma' q}\sim\sum_p\bar\psi_{\sigma p}\psi_{\sigma' p+q}$, and the third in the Cooper channel $\hat\rho_{{\rm c},\sigma\sigma' q}\sim\sum_p\bar\psi_{\sigma p}\bar\psi_{\sigma' -p+q}$. One thus winds up with an effective theory that contains three independent slow Hubbard–Stratonovich fields. (Notice that the decoupling fields in the exchange and in the Cooper channel explicitly carry a spin–structure.)

After this digression on the principles of the Hubbard–Stratonovich transformation, let us now return to the discussion of the electron gas.

At the expense of introducing a second field, the Hubbard-Stratonovich transformation provides an action quadratic in the fermion fields. In this case, the fermion integration can be undertaken exactly. Making use of the Gaussian functional integral (4.19), one obtains

$$\mathcal{Z} = \int D\phi\, e^{-\frac{1}{8\pi}\sum_q \phi_q \mathbf{q}^2\phi_{-q}}\det\left[\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi\right]^2,$$

where the factor of two accounts for the spin degeneracy.

The standard procedure to deal with the determinants generated at intermediate stages of the manipulation of a field integral is to simply re–exponentiate them. This is achieved by virtue of the identity,

$$\boxed{\ln\det\hat A = \ \mathrm{tr}\ \ln\hat A} \tag{5.4}$$

valid for arbitrary (non–singular) operators $\hat A$.[6] Thus, the quantum partition function

[6] Eq. (5.4) is readily established by switching to an eigenbasis whereupon one obtains $\ln\det\hat A = \sum_a \ln\epsilon_a = \mathrm{tr}\,\ln\hat A$, where ϵ_a are the eigenvalues of $\hat A$ and we have used the fact that the eigenvalues of $\ln\hat A$ are $\ln\epsilon_a$.

takes the form $\mathcal{Z} = \int D\phi\, e^{-S[\phi]}$, where

$$S[\phi] = \frac{1}{8\pi}\sum_q \phi_q \mathbf{q}^2 \phi_{-q} - 2\mathrm{tr}\ \ln\left[\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi\right]. \tag{5.5}$$

This is as far as purely formal exact manipulations can carry us. We have managed to trade the integration over the interacting Grassmann field ψ_σ for an integration over an auxiliary field ϕ; a field that we believe encapsulates the relevant degrees of freedom of the model. This completes steps 1, 2, and 3 of the general programme outlined above.

Ordinarily, the next step in the programme is to subject the action to a stationary phase analysis, i.e. to seek solutions of the set of saddle-point equations such that

$$\forall q = (\mathbf{q} \neq 0, \omega): \qquad \frac{\delta S[\phi]}{\delta \phi_q} \stackrel{!}{=} 0\,.$$

Such a solution $\phi(\mathbf{x}, t) \leftrightarrow \phi_q$ is commonly referred to as a **mean-field**. This terminology can be understood by inspection of the argument of the 'tr ln' above. The structure $\hat{\mathbf{p}}^2/2m - \mu + ie\phi$, where ϕ is a fixed configuration (to be determined by solving the saddle–point equations), resembles the Hamiltonian operator of particles subject to some background potential, or 'mean' field. The notation on the left hand side of the saddle-point equations indicates that our original interaction $V(\mathbf{q})$ and, therefore, the decoupling field ϕ do not possess a zero momentum mode (a consequence of charge neutrality).

However, in the present case, since the interaction is considered weak, we may anticipate that the solution to the saddle-point variation is the trivial one, viz. $\phi = 0$ — an assumption that we may check self-consistently. In this case, step 4 of the general programme may be considered as achieved and we may turn to explore fluctuations around $\phi = 0$. Since the mean-field solution vanishes, it makes no sense to introduce new notation, i.e. we will denote the fluctuations again by the symbol ϕ.

As regards the first term in the action (5.5), it has already a quadratic form. The logarithmic contribution can be expanded as if we were dealing with a function (again, a consequence of the trace), i.e. setting

$$\hat{G}^{-1} \equiv \hat{G}_0^{-1} + ie\phi,$$

$\hat{G}_0^{-1} \equiv \partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu$ is the momentum and frequency diagonal operator whose matrix elements give the free Green function of the electron gas, we may express

$$\begin{aligned}\mathrm{tr}\ln\hat{G}^{-1} &= \mathrm{tr}\ln(\hat{G}_0^{-1} + ie\phi) = \mathrm{tr}\ln\hat{G}_0^{-1} + \mathrm{tr}\ln(1 + ie\hat{G}_0\phi)\\ &= \mathrm{tr}\ \ln\hat{G}_0^{-1} + ie\mathrm{tr}\,(\hat{G}_0\phi) + \frac{e^2}{2}\mathrm{tr}\,(\hat{G}_0\phi\hat{G}_0\phi) + \ldots.\end{aligned}$$

Being ϕ–independent, the first term generates an overall constant multiplying the functional integral, viz. a constant that must describe the non–interacting content of the theory. Indeed, one may note that $e^{2\mathrm{tr}\,\ln\hat{G}_0^{-1}} = e^{-2\mathrm{tr}\,\ln\hat{G}_0} = (\det\hat{G}_0^{-1})^2 \equiv \mathcal{Z}_0$ is just the partition function of the non-interacting electron gas. Linear in $\hat{\phi}$, the second term of the expansion must, by virtue of the mean-field analysis, vanish. (Afterall, we are expanding around an extremum! To this end, one may note that $\mathrm{tr}\,(\hat{G}_0\phi) = \sum_q G_0(q)\phi_{q=0} = 0$.)

The third term is the interesting one. Remembering that ϕ couples to the theory as a potential, this term describes how potential flucutations are affected by the presence of the electron gas, i.e. it must encode the *screening* of the electromagnetic field by the electron degrees of freedom.

To resolve this connection, let us make the momentum dependence of the second–order term explicit (exercise[7]):

$$\frac{e^2}{2}\mathrm{tr}\,(\hat{G}_0\phi\hat{G}_0\phi) = \frac{e^2}{2\beta L^3}\sum_{p,q} G_0(p+q)\phi_q G_0(p)\phi_{-q} = \frac{e^2}{4}\sum_q \Pi(q)\phi_q\phi_{-q}\,,$$

where, setting $\xi_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m} - \mu$,

$$\boxed{\Pi(q) = \sum_p G_0(p)G_0(p+q) = \frac{2}{\beta L^3}\sum_{\omega_n,\mathbf{p}} \frac{1}{-i\omega_n + \xi_{\mathbf{p}}}\;\frac{1}{-i\omega_n - i\omega_m + \xi_{\mathbf{p}+\mathbf{q}}}}$$

Collecting together the bare photon action with this expansion, to leading order in e, the quantum partition function takes the form

$$\mathcal{Z} = \mathcal{Z}_0 \int D\phi\, e^{-S[\phi]},$$

where the effective action for the electromagnetic field ϕ is given by

$$\boxed{S[\phi] = \frac{1}{2}{\sum_q}' \frac{1}{D(q)}|\phi_q|^2 + O(e^4)}$$

This result has a clear physical interpretation: the interaction of the electron gas with the electromagnetic field induces a modified or **screened Coulomb interaction** (see Fig. 5.3),

$$\boxed{D(\omega_m,\mathbf{q}) = \frac{1}{\epsilon(\omega_m,\mathbf{q})}\frac{4\pi}{\mathbf{q}^2}, \qquad \epsilon(\omega_n,\mathbf{q}) = 1 - \frac{4\pi e^2}{\mathbf{q}^2}\Pi(\omega_m,\mathbf{q})}$$

where $\epsilon(\omega_m,\mathbf{q})$ is the energy and momentum dependent effective **dielectric function**. This perturbative result, which is known in the literature as the **Random Phase Approximation (RPA)**, amounts to treating the long-range part of the Coulomb interaction as an "external" polarisation field, and the correction to the dielectric function, $(4\pi e^2/\mathbf{q}^2)\Pi(\omega_m,\mathbf{q})$, is known as the **screened polarisability**. To explore the dielectric properties of the interacting electron gas it is necessary to understand the frequency and momentum dependence of the density-density response function (5.6). To do so we must first learn how to perform Matsubara frequency summations.

▷ INFO. Frequently, in working with imaginary time field integrals one often needs to perform **Matsubara frequency summations**. At low temperatures it can be argued that

[7] Hint: Consider the strategic incorporation of the resolution of identity $1 = \sum_q |q\rangle\langle q|$ underneath the trace.

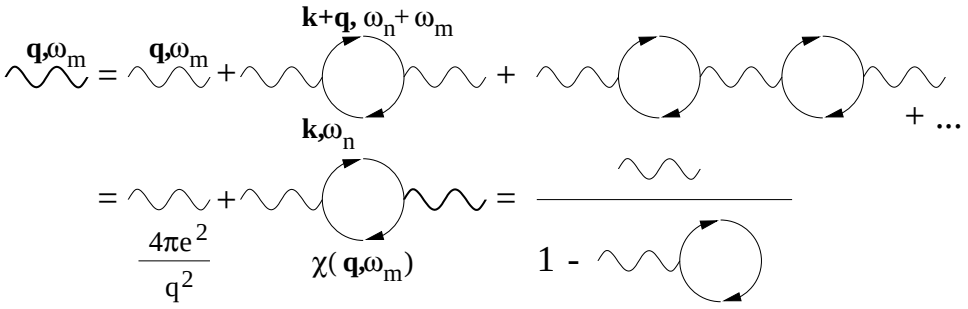


Figure 5.3: The modified screened Coulomb interaction, $D(\omega_m, \mathbf{q})$ can be viewed as the summation of an infinite 'diagrammatic' series expansion in the interaction: The bare Coulomb interaction vertex is 'dressed' by repeated particle-hole excitations of the electron gas. The corresponding summation of the geometric series (known as a **Dyson equation**) is shown schematically and can be compared to Eq. (5.6).

the spacing $2\pi/\beta$ between neighbouring Matsubara frequencies scales to zero which legitimates changing the summations into integrals. However, as we have seen previously, there exists an alternative way of evaluating the sums which not only keeps the finite temperature content of the theory but is also more efficient *even* in the limit of zero temperature.

Referring to our ealier discussion for details, the basic idea behind the standard scheme of evaluating frequency summations is to introduce a complex auxiliary function $g(z)$ that has simple poles at $z = i\omega_n$. The sum $\sum_n f(i\omega_n)$ one wishes to compute then emerges as the sum of residues obtained by integrating the product gf along a suitably chosen path C in the complex plane. The choice of both the function g and the integration contour C depend on the structure of the sum in which one is interested (convergence and analyticity properties of f, etc.). In the present case, the screened polarisability (5.6),

$$g(z) = \frac{\beta}{\exp(\beta z) + 1}, \qquad f(z) \equiv \frac{1}{z - \mu + \epsilon} \; \frac{1}{z - \mu + \epsilon'},$$

and C is a circular contour of infinite radius in the complex plane (see Fig. 5.4). We are therefore led to consider the integral

$$I \equiv \int_C dz \frac{\beta}{\exp(\beta z) + 1} \frac{1}{z - \mu + \epsilon} \; \frac{1}{z - \mu + \epsilon'}. \tag{5.6}$$

Two important observations can be made without explicit computation: (i) The integral exists (the integrand decays sufficiently fast in all directions for $|z| \to \infty$), and (ii) $I = 0$ (the reason being that for $|z| \to \infty$, the product $fg < z^{-\gamma}$, where $\gamma > 1$). Thus the integral of fg over a circle (radius $\sim z$) scales to zero as the radius $\to \infty$. On the other hand, the integral along C gives the sum over the residues of all enclosed poles. The function fg has poles at the Matsubara frequencies $i\omega_n$ and poles on the real axis at $z = \mu - \epsilon$ and $z = \mu - \epsilon'$. Hence,

$$0 = \int_C dz (fg)(z) = 2\pi i \left(\sum_n \text{Res } (fg)(i\omega_n) + \text{Res } (fg)(\mu - \epsilon) + \text{Res } (fg)(\mu - \epsilon') \right).$$

At the Matsubara frequencies, f is analytic and g has, by construction, unit residue. Thus

$$\text{Res } (fg)(i\omega_n) = -f(i\omega_n).$$

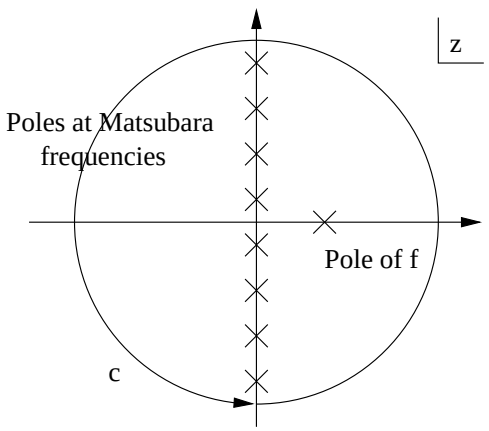


Figure 5.4: Complex integration contour employed in calculating the sum (5.6).

At $z = \mu - \epsilon$, f has a simple pole, whereas g is analytic, i.e.

$$\text{Res } (fg)(\mu - \epsilon) = \frac{g(\mu - \epsilon)}{(\epsilon' - \epsilon)}.$$

Combined with the pole at $z = \mu - \epsilon'$, and making use of the identity $e^{i\beta\omega_n} = 1$, we obtain

$$\Pi(\omega_m, \mathbf{q}) = \frac{2}{L^3} \sum_{\mathbf{k}} \frac{n_{\rm F}(\xi_{\mathbf{k}}) - n_{\rm F}(\xi_{\mathbf{k}+\mathbf{q}})}{i\omega_m + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}} \tag{5.7}$$

where we have made use of the fact that, on the real axis, the auxiliary function g is proportional to the Fermi-Dirac distribution function,

$$n_{\rm F}(\xi_{\mathbf{k}}) = \frac{1}{e^{\beta(\mu - \epsilon_{\mathbf{k}})} + 1}. \tag{5.8}$$

To analyse the screened Coulomb interaction $D(\omega_n, \mathbf{q})$ we consider Eq. (5.7) for the density-density response function, and divide our consideration into two limits:

▷ **Static Limit** ($|\omega_n| \ll k_F|\mathbf{q}|/m$)

For frequencies small as compared to the momentum transfer (and temperatures $T \ll \mu$), the response function converges to the static limit

$$\frac{\Pi(0, \mathbf{q})}{2} \simeq \frac{}{L^3} \sum_{\mathbf{k}} \frac{\mathbf{q} \cdot \partial_{\mathbf{k}} n_{\rm F}(\xi_{\mathbf{k}})}{\mathbf{q} \cdot \partial_{\mathbf{k}} \xi_{\mathbf{k}}} \simeq \int \frac{d^3k}{(2\pi)^3} \partial_{\xi_{\mathbf{k}}} n_{\rm F}(\xi_{\mathbf{k}}) = \int_0^\infty d\epsilon \nu(\epsilon) \partial_\epsilon n_{\rm F}(\epsilon - \mu) \simeq -\nu(\mu),$$

where here we have made use of the fact that $\xi_{\mathbf{k}}$ depends only on $|\mathbf{k}|$, and we have deployed the continuum limit, $\frac{1}{L^3} \sum_{\mathbf{k}} \mapsto \int \frac{d^3k}{(2\pi)^3} = \int_0^\infty d\epsilon \nu(\epsilon)$ with $\nu(\epsilon) \equiv 1/|\nabla_{\mathbf{k}} \xi_{\mathbf{k}}| = 2mk/(2\pi)^2$ the density of states. From this result, one obtains the screened Coulomb interaction

$$D(q) = \frac{1}{\frac{\mathbf{q}^2}{4\pi} + 2e^2\nu(\mu)}$$

When transformed back to real space, one obtains the effective static screened Coulomb interaction

$$\boxed{D(\mathbf{r}) = \frac{e^2}{|\mathbf{r}|} e^{-|\mathbf{r}|/\lambda_{\rm TF}}}$$

where $\lambda_{\rm TF} = (8\pi e^2 \nu(\mu))^{1/2}$ defines the **Thomas-Fermi screening length**. Physically, the bare Coulomb interaction is screened by the collective fluctuations of the electron gas.

▷ **High Frequency Limit** ($|\omega_n| \gg k_F|\mathbf{q}|/m$)

By contrast, in the high frequency limit, the density-density response function takes the form

$$\Pi(\omega_m, \mathbf{q}) \simeq -\frac{2}{L^3}\sum_{\mathbf{k}} \frac{\mathbf{q}\cdot\partial_{\mathbf{k}} n_{\rm F}(\xi_{\mathbf{k}})}{i\omega_m - \mathbf{q}\cdot\partial_{\mathbf{k}}\xi_{\mathbf{k}}} \simeq -\int \frac{d^3k}{(2\pi)^3}\frac{2}{i\omega_m}\left(1 + \frac{\mathbf{q}\cdot\mathbf{k}}{im\omega_m}\right)\mathbf{q}\cdot\partial_{\mathbf{k}} n_{\rm F}(\xi_{\mathbf{k}})$$
$$\overset{\text{by parts}}{=} -\int \frac{d^3k}{(2\pi)^3}\frac{2\mathbf{q}^2}{m\omega_m^2} n_{\rm F}(\xi_{\mathbf{k}}) = -\frac{1}{(2\pi)^3}\frac{4}{3}\pi k_F^3 \frac{2\mathbf{q}^2}{m\omega_m^2} = -\frac{N}{2L^3}\frac{2\mathbf{q}^2}{m\omega_m^2} = -\frac{n\mathbf{q}^2}{m\omega_m^2},$$

where $n = N/L^d$ denotes the total number density. Applying the analytic continuation to real frequencies, $i\omega_n \to \omega + i0$, we obtain

$$\lim_{m\omega/k_F|\mathbf{q}|\to\infty} D(\omega, \mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2}\left[1 - \frac{\omega_p^2}{\omega^2}\right]^{-1},$$

where $\omega_p = 4\pi e^2 n/m$ represents the **Plasma frequency**. At high frequencies the dielectric response of the system is sensitive to the plasma oscillations of the background electron charge. In particular, for $\omega = \omega_p$, the collective excitations become undamped.

▷ Ground State Energy

Finally, from the partition function, it is possible to obtain an estimate of the ground state energy of the interacting electron gas.

$$\lim_{\beta\to\infty} \mathcal{Z} \sim e^{-\beta E_{\rm g.s.}}.$$

In the RPA approximation, performing the functional integral over the Gaussian action in ϕ, we obtain

$$E_{\rm g.s.} = E_{\rm g.s.}(e=0) - \frac{1}{2\beta}\sum_{\omega_n,\mathbf{q}} \ln D(\omega_n, \mathbf{q}).$$

where $E_{\rm g.s.} \equiv -\ln \mathcal{Z}_0/\beta = 3n\mu/5$ is the ground state energy of the free electron gas. This was the formula derived by Gell-Mann and Brückner from which, after some extensive algebra (exercise!), one obtains the high density ($r_s \ll 1$) expansion

$$E_{\rm g.s.} = n\left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.622\ln r_s - 0.142\right)\text{Ryd}.$$

This concludes our preliminary analysis of the screening properties of the weakly interacting electron gas. By employing the coherent state path integral, we were (implicitly) able to establish the stability of the non-interacting ground state, determine the modified screened Coulomb interaction, and identify plasma oscillations. In the following section, we will use the path integral to study the weakly interacting Bose gas and the phenomenon of superfluidity.

5.3 Bose–Einstein Condensation and Superfluidity

Previously, we have considered the influence of weak Coulomb interaction on the properties of the electron gas. In the following, our goal will be to consider the phases realised by a weakly interacting Bose gas. To this end, let us introduce the quantum partition function $\mathcal{Z} = \int D(\bar{\psi}, \psi)\, e^{-S[\bar{\psi},\psi]}$, where

$$S[\bar{\psi}, \psi] = \int d^d r \int d\tau \left[\bar{\psi}(\mathbf{r}, \tau)(\partial_\tau + \hat{H}_0 - \mu)\psi(\mathbf{r}, \tau) + \frac{g}{2}(\bar{\psi}(\mathbf{r}, \tau)\psi(\mathbf{r}, \tau))^2 \right]. \qquad (5.9)$$

Here ψ represents a complex field subject to the periodic boundary condition $\psi(\mathbf{r}, \beta) = \psi(\mathbf{r}, 0)$. The functional integral $\mathcal{Z}$ describes the physics of a system of bosonic particles in d–dimensions subject to a repulsive contact interaction of strength $g > 0$. For the moment the specific structure of the one–body operator $\hat{H}_0$ need not be specified. The most remarkable phenomena displayed by systems of this type are Bose–Einstein condensation and superfluidity. However, contrary to a widespread belief, these two effects do not mutually depend on each other: Superfluidity can arise without condensation and *vice versa*. We begin our discussion with the more elementary of the two phenomena.

5.3.1 Bose–Einstein Condensation

As may be recalled from elementary statistical mechanics, at sufficiently low temperatures, the ground state of a bosonic system can involve the condensation of a macroscopic fraction of particles into a single state. This phenomenon, predicted in a celebrated work by Einstein[8] is known as Bose–Einstein condensation. To see how this phenomenon is born out of the functional integral formalism, let us temporarily switch off the interaction and turn to the basis in which the one–particle Hamiltonian is diagonal. Expressed in the frequency representation, the partition function of the non–interacting system is given by,

$$\mathcal{Z}_0 \equiv \mathcal{Z}\Big|_{g=0} = \int D(\bar{\psi}, \psi)\, \exp\left[-\sum_{an} \bar{\psi}_{an} \left(-i\omega_n + \epsilon_a - \mu \right) \psi_{an} \right].$$

Albert Einstein 1879–1955: 1921 Nobel Laureate in Physics "for his services to theoretical physics, and especially for his discovery of the law of the photoelectric effect". His work on the low temperature behaviour of the bosonic quantum gas is published in A. Einstein, *Quantentheorie des einatomigen idealen Gases*, Sitzungsber. Preuss. Akad. Wiss. **1925**, 14 (1925).

[8]

Without loss of generality, we may assume that the eigenvalues $\epsilon_a \geq 0$ are positive with a ground state $\epsilon_0 = 0$.[9] (In contrast to the fermionic systems discussed above, we should not have in mind low energy excitations superimposed on high energy microscopic degrees of freedom. Here, everything will take place in the vicinity of the ground state of the microscopic single–particle Hamiltonian.) Furthermore, we note that, to ensure stability, the chemical potential determining the number of particles in the system must be negative for, otherwise, the Gaussain weight corresponding to the low–lying states $\epsilon_a < -\mu$ would change sign resulting in an ill–defined theory.

From our discussion of section 4.2.1 we recall that the number of particles in the system is set by the relation ($k_B = 1$)

$$N(\mu) = -\frac{\partial F}{\partial \mu} = T\frac{\partial}{\partial \mu}\ln \mathcal{Z} = T\sum_{na}\frac{1}{i\omega_n - \epsilon_a + \mu} = \sum_a n_{\rm B}(\epsilon_a)\,,$$

where, as usual, $n_{\rm B}(\epsilon) = (e^{\beta(\epsilon-\mu)} - 1)^{-1}$ denotes the Bose distribution. For a given number of particles, this equation determines the temperature dependence of the chemical potential, $\mu(T)$. As the temperature is reduced, the distribution function controlling the population of individual states decreases. Since the number of particles must be kept constant, this scaling must be counter–balanced by a corresponding increase in the chemical potential.

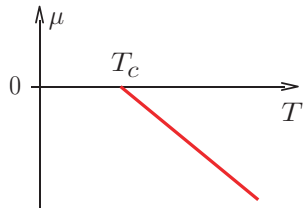


Figure 5.5: Schematic plot showing the variation of the chemical potential as a function of temperature. Note that, for $T < T_c$, the chemical potential remains pinned at zero.

Below a certain critical temperature T_c, even the maximum value of the chemical potential, $\mu = 0$, will not suffice to keep the distribution function $n_{\rm B}(\epsilon_{a\neq 0})$ large enough to accomodate all particles in the states of non–vanishing energy, viz. $\sum_{a>0} n_{\rm B}(\epsilon_a)|_{\mu=0} \overset{T<T_c}{\equiv} N_1 < N$. I.e. below the critical temperature, the chemical potential stays constant at $\mu = 0$ (see the figure). As a result, a macroscopic number of particles $N - N_1$ must accumulate in the single–particle ground state: **Bose–Einstein condensation**.

▷ EXERCISE. For a three–dimensional free particle spectrum, $\epsilon_k = \hbar^2 k^2/2m$, show that the critical temperature is set by $T_c = \frac{c_0\hbar^2}{ma^2}$, where $a = \rho^{-1/3}$ is the average interparticle spacing, and c_0 is a constant of order unity. Show that for temperatures $T < T_c$, the density of particles in the condensate ($\mathbf{k} = 0$) is given by $\rho_0(T) = \rho[1 - (\frac{T}{T_c})^{3/2}]$.

▷ INFO. Since its prediction in the early 20s, the phenomenon of Bose–Einstein condensation has been a standard component of undergraduate texts. However, it took some seven decades

[9] The chemical potential μ can always be adjusted so as to meet this condition.

before the condensation of bosonic particles was directly[10] observed in experiment. The reason for this delay is that the critical condensation temperature of particles that are comfortably accessible to experiment — atoms — is absurdly low.

In 1995 the groups of Cornell and Wieman at Colorado University and, soon after, Ketterle at MIT succeeded in cooling a system of rubidium atoms down to temperatures of 20 billionths(!) of a Kelvin.[11] To reach these temperatures, a gas of rubidium atoms was caught in a magnetic trap, i.e. a configuration of magnetic field gradients that couple to the magnetic moments of the atoms so as to keep the system spatially localized (see the schematic).

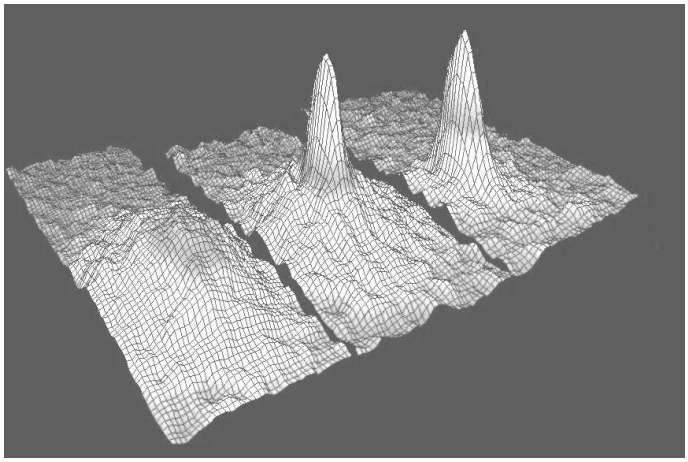


Figure 5.6: Spectroscopic images of a gas of atoms at 400nK (left), 200nK (middle), and 50nK (right). The peak in the density distribution signals the onset of condensation. Courtesy of JILA institute, University of Colorado

The gas of atoms was then brought to a temperature of $\mathcal{O}(10^{-5})$K — still much too hot to condense — by 'laser cooling'; crudely speaking, a technique where atoms, subjected to a suitably adjusted ray of monochromatic light, may transmit more of their kinetic energy to the photons than they get back. To lower the temperature still further, the principle of 'evaporative cooling' was applied: By lowering the potential well of the trap, a fraction of the atoms, namely those with large kinetic energy, is allowed to escape. The remaining atoms have a low kinetic energy and, therefore, a low temperature. What sounds like a simple recipe actually represents a most delicate experimental procedure. (For example, if the trap potential is lowered too strongly, all atoms escape and there is nothing left to condense. If, on the other hand, trapping is too strong, the atoms remain too hot, etc.) However, after more than a decade of intensive experimental preparation, the required temperatures have been reached.

Spectroscopic images of the Bose–Einstein condensation process are shown in the figure (courtesy of the JILA institute, University of Colorado) for three values of temperature (400 nK, 200 nK, and 50 nK from left to right). The peak in the density distribution signals the onset of condensation. On lowering the temperature, one may observe the transition to a condensed phase by monitoring the formation of a peak in the density distribution. The preparation of

[10]Here, by 'direct' we refer to the controlled preparation of a state of condensed massive bosonic particles. There are numerous 'indirect' manifestations of condensed states, e.g. the anomalous properties of the Helium liquids at low temperatures, or of Cooper–pair condensates in superconductors.

[11]M. H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E. A. Cornell, *Observation of Bose–Einstein Condensation in a Dilute Atomic Vapor*, Science **269**, 198 (1995).

a Bose condensed state of matter was recognized with the award of the 2001 Nobel prize in physics. Since 1995, research on atomic condensates has blossomed into a broad arena of research. Already, it is possible to prepare complex states of Bose condensed matter such as atomic vortices in rotating Bose–Einstein condensates, condensates in different dimensionalities, or even an artificial crystalline state of matter. A detailed discussion of these interesting developments is beyond the scope of the present text.

With this background, let us now try to understand how the phenomenon of Bose–Einstein condensation can be implemented into the functional integral representation. Evidently, the characteristics of the condensate will be described by the zero field component $\psi_0(\tau)$. The problem with this zero mode is that, below the condensation transition, its action apears to be unbound: both the chemical potential and the eigenvalue are zero. This means that the action of the zero Matsubara component $\psi_{0,0}$ vanishes. We will deal with this difficulty in a pragmatic way. That is, we will not treat $\psi_0(\tau)$ as an integration variable but rather as a time–independent Lagrange multiplier to be used to fix the number of particles below the transition. More precisely, we introduce a reduced action of the form

$$S_0[\bar{\psi}_0, \psi_0] = -\bar{\psi}_0 \beta\mu \psi_0 + \sum_{a\neq 0,n} \bar{\psi}_{an} \left(i\omega_n + \epsilon_a - \mu\right) \psi_{an} \,,$$

where we did not yet set $\mu = 0$ (since we still need μ as a differentiation variable). To understand the rational behind this simplification one may note that

$$N = -\partial_\mu F_0|_{\mu=0^-} = T\partial_\mu \ln \mathcal{Z}_0|_{\mu=0^-} = \bar{\psi}_0\psi_0 + T\sum_{a\neq 0,n} \frac{1}{i\omega_n - \epsilon_a} = \bar{\psi}_0\psi_0 + N_1 \qquad (5.10)$$

determines the number of particles. According to this expression, $\bar{\psi}_0\psi_0 = N_0$ sets the number of particles in the condensate. Now, what enables us to regard ψ_0 as a time–independent field? Remembering the construction of the path integral, we note that the introduction of time–dependent fields, or 'time slicing' was necessitated by the fact that the operators appearing in the Hamiltonian of a quantum theory do not, in general, commute. (Otherwise we could have decoupled the expression $\mathrm{tr}\,(e^{-\beta(\hat{H}-\mu\hat{N})(a^\dagger,a)}) \simeq \int d(\bar{\psi},\psi) e^{-\beta(H-\mu N)(\bar{\psi},\psi)}$ in terms of a single coherent state resolution, i.e. a 'static' configuration). Reading this observation in reverse, we conclude that the dynamic content of the field integral represents the quantum character of a theory. (Alluding to this fact, the temporal fluctuations of field variables are often referred to as **quantum fluctuations**.) Conversely, *a static approximation in a field integral $\psi(\tau) = \psi_0 =$ const. amounts to replacing a quantum degree of freedom by its classical approximation.*
(In order to distinguish them from quantum, fluctuations in the 'classical' static sector of the theory are called **thermal fluctuations**.) To justify the approximation of $a_0 \leftrightarrow \psi_0$ by a classical object, notice that, upon condensation, $N_0 = \langle a_0^\dagger a_0\rangle$ will assume 'macroscopically large' values. On the other hand, the commutator $[a_0, a_0^\dagger] = 1$, continues to be of $\mathcal{O}(1)$. It thus seems to be legitimate to neglect all commutators of the zero operator a_0 in comparison with its expectation value — a classical approximation.[12]

[12]Notice the similarity of that reasoning to the arguments employed in connection with the semi–

Now, we are still left with the problem that the ψ_0–integration appears to be un–defined. The way out is to remember that the partition function should extend over those states that contain an (average) number of N particles. That is, Eq. (5.10) has to be interpreted as a relation that fixes the modulus $\bar{\psi}_0\psi_0$ so as to adjust the appropriate value of N. (For a more rigorous discussion of the choice of the thermodynamic variables in the present context, we again refer to Ref.[1].)

5.3.2 The Weakly Interacting Bose Gas

Now, with this background, let us restore the interaction focussing on a small but finite coupling constant g. To keep the discussion concrete, we specialize to the case of a free single-particle system, $\hat{H}_0 = \hat{\mathbf{p}}^2/2m$. (Notice that the ground state wavefunction of this system describes a spatially constant zero momentum state.) By adiabatic continuity we expect that much of the picture developed above will survive generalization to non–zero interaction strengths. In particular, the ground state, which in the case under consideration corresponds to a temporally and spatially constant mode ψ_0, will continue to be macroscopically occupied. Under these circumstances, the dominant contribution to the action will again come from the classical ψ_0 sector:

$$TS[\bar{\psi}_0, \psi_0] = -\mu\bar{\psi}_0\psi_0 + \frac{g}{2L^d}(\bar{\psi}_0\psi_0)^2 \,. \tag{5.11}$$

Crucially, the stability of the action is now guaranteed by the interaction vertex, no matter how small is $g > 0$ (see the schematic plot of the action in the figure). Accordingly, we will no longer treat ψ_0 as a fixed parameter but rather as an ordinary intergration variable. Integration over all field components will produce a partition function $\mathcal{Z}(\mu)$ that depends parametrically on the chemical potential. As usual in statistial physics, the latter can then be employed to fix the particle number. (Notice that, vis–a–vis aspects of thermodynamics, the interacting system appears to behave more 'naturally' than its ideal, non–interacting approximation. This reflects a general feature of bosonic systems; interactions 'regularize' a number of pathological features of the ideal gas.)

Returning to the ψ_0–integration, we observe that, for low enough temperatures, the problem is an ideal candidate for saddle–point analysis. Variation of the action with respect to ψ_0 obtains

$$\psi_0 \left(-\mu + \frac{g}{L^d}\bar{\psi}_0\psi_0\right) = 0.$$

This equation is solved by any constant complex field configuration ψ_0 with modulus $|\psi_0| = \sqrt{\mu L^d/g} \equiv \gamma$. Inspite of its innocent appearance, this equation reveals much about the nature of the system:

---

classical treatment of spin systems in the limit of large S (section 2.2.4). Unfortunately, the actual state of affairs with the classical treatment of the condensate is somewhat more complex than the simple argument above suggests. (For a good discussion, see Ref. [1].) However, the net result of a more thorough analysis, i.e. an integration over all dynamically fluctuating components $\psi_{0,n\neq 0}$, shows that the treatment of ψ_0 as classical represents a legitimate approximation.

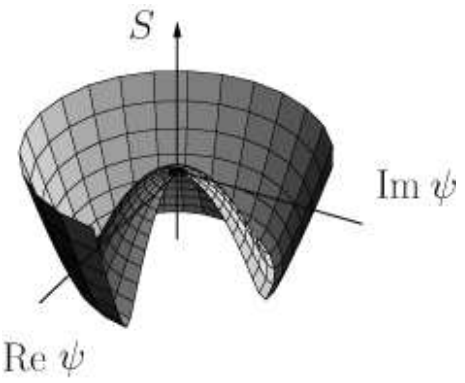


Figure 5.7: The action $S[\bar{\psi}_0, \psi_0]$ shown as a function of real and imaginary part of the condensate field (part removed for clarity). The most important features of the action are (a) the existence of a degenerate minimum determined by the set of solutions of the equation $\partial_{|\psi_0|} S = 0$, and (b) the large amplitude asymptotics $\sim \beta g |\psi_0|^4$ stabilizing the ψ_0-integration.

- ▷ For $\mu < 0$ (i.e. above the condensation threshold of the non–interacting system), the equation exhibits only the trivial solution $\psi_0 = 0$. This means that no stable condensate amplitude exists.
- ▷ Below the condensation threshold (i.e. for $\mu \geq 0$),[13] the equation is solved by any configuration with $|\psi_0| = \gamma \equiv \sqrt{\mu L^d / g}$. (Notice that $\bar{\psi}_0 \psi_0 \propto L^d$, reflecting the macroscopic population of the ground state.)
- ▷ The equation couples only to the modulus of ψ_0. I.e. the solution of the stationary phase equation is continuously degenerate: Each configuration $\psi_0 = \gamma \exp(i\phi), \phi \in [0, 2\pi]$ is a solution.

For our present discussion, the last of the three aspects mentioned above is the most important. It raises the question as to which of the configurations $\psi_0 = \gamma \exp(i\phi)$ is the 'right' one?

Without loss of generality, we may chose $\psi_0 = \gamma \in \mathbb{R}$ as a reference configuration for our theory. This choice amounts to selecting a particular minimum lying in the 'mexican hat' profile of the action shown above. However, it is clear that an expansion of the action around that minimum will be singular: Fluctuations $\psi_0 \to \psi_0 + \delta\psi$ that do not leave the azimuthally symmetric well of degenerate minima do not change the action and, therefore, have vanishing expansion coefficients. As a result, in the present situation, we will not be able to implement a simple scheme viz. 'saddle–point plus quadratic fluctuations'. (There is nothing that constrains the deviations $\delta\psi$ to be small.) The integral over fluctuations around the mean–field configuration has to be undertaken in a more careful way.

▷ Info. The mechanism encoutered here is one of **spontaneous symmetry breaking**. To understand the general principle, consider an action $S[\psi]$ with a global continuous symmetry

[13] Due to the stabilization of the zero mode integration by the interaction constant, $\mu \leq 0$ is no longer a strict condition.

under some transformation g (not to be confused with the afore mentioned coupling constant of the Bose gas): Specifically, the action remains invariant under a global transformation of the fields such that, $\forall i \in M : \psi_i \to g\psi_i$, where M is known as the "base manifold", i.e. $S[\psi] = S[g\psi]$. The transformation is 'continuous' in the sense that g takes values in some manifold, typically a group G.

Examples: The action of a Heisenberg ferromagnet is invariant under **rotation** of all spins simultaneously by the same amount, $\mathbf{S}_i \to g\mathbf{S}_i$. In this case, $g \in G = \mathrm{O}(3)$, the three–dimensional group of rotations. The action of the displacement fields $\mathbf{u}$ describing elastic deformations of a solid (phonons) is invariant under simultaneous **translation** of all displacements $\mathbf{u}_i \to \mathbf{u}_i + \mathbf{a}$, i.e. the symmetry manifold is the the d–dimensional translation group $G \simeq \mathbb{R}^d$. In the example above, we encountered a U(1) symmetry under phase multiplication $\psi_0 \to e^{i\phi}\psi_0$. This phase freedom expresses the **global gauge symmetry** of quantum mechanics under transformation by a phase, a point we will discuss in more detail below.

Now, given a theory with globally G invariant action, two scenarios are conceivable: Either the ground states share the invariance properties of the action or they do not. The two alternatives are illustrated in the figure for the example of the Bose system. For $\mu > 0$, the action $S[\bar{\psi}_0, \psi_0]$ has a single ground state at $\psi_0 = 0$. This state is trivially symmetric under the action of $G = \mathrm{U}(1)$. However, for negative μ, i.e. in the situation discussed above, there is an entire manifold of degenerate ground states, defined through the relation $|\psi_0| = \gamma$. These ground states transform into each other under the action of the gauge group. However, none of them is individually invariant.

With the other examples mentioned above, the situation is similar. For symmetry groups more complex than the one–dimensional manifold U(1), the ground states will, in general, be invariant under transformation by the elements of a certain subgroup $H \subseteq G$ (that includes the two extremes $H = \{\mathbf{1}\}$ and $H = G$). For example, below the transition temperature, the ground state of the Heisenberg magnet will be given by (domainwise) aligned configurations of spins. Assuming that the spins are oriented along the z–direction, the ground state is invariant under the abelian subgroup $H \subset \mathrm{O}(3)$ containing all rotations around the z–axis. However, invariance under the full rotation group is manifestly broken. Solids represent states where the translation symmetry is fully broken, i.e. all atoms collectively occupy a fixed pattern of spatial positions in space, $H = \{\mathbf{1}\}$, etc.

Inspite of the undeniable existence of solids, magnets, and Bose condensates of definite phase, the notion of a ground state that does not share the full symmetry of the theory may appear paradoxical, or at least 'unnatural'. For example, even if any particular ground state of the 'Mexican hat' potential shown in the figure above 'breaks' the rotational symmetry, shouldn't all these states enter the partition sum with equal statistical weight, such that the net outcome of the theory is again fully symmetric?

To understand why symmetry breaking is a 'natural' and observable phenomenon, it is instructive to perform a gedanken experiment: To this end, consider the partition function of a classical[14] ferromagnet,

$$\mathcal{Z} = \mathrm{tr}\left(e^{-\beta(H - \mathbf{h}\cdot\sum_i \mathbf{S}_i)}\right),$$

where H is the rotationally invariant part of the energy functional and $\mathbf{h}$ represents a weak external field. (Alternatively, we can think of $\mathbf{h}$ as an internal field, caused by a slight structural imperfection of the system.) In the limit of vanishing field strength, the theory becomes

[14] The same argument can be formulated for the quantum magnet.

manifestly symmetric. Symbolically,

$$\lim_{N\to\infty}\lim_{h\to 0}\mathcal{Z} \longrightarrow \text{rot. sym.}\,,$$

where the limit $N \to \infty$ serves as a mnemonic indicating that we consider systems of macroscopic size. However, keeping in mind the fact that the model ought to describe a physical magnetic system, the order of limits taken above appears questionable. Since the external perturbation couples to a macroscopic number of spins, a more natural description of an 'almost' symmetric situation would be

$$\lim_{h\to 0}\lim_{N\to\infty}\mathcal{Z} \longrightarrow\ ?$$

The point is that the two orders of limits lead to different results. In the latter case, for any $\mathbf{h}$, the $N \to \infty$ system is described by an explicitly symmetry broken action. No matter how small the magnetic field, the energetic cost to rotate $N \to \infty$ spins against the field is too high, i.e. the ground state $|\mathbf{S}\rangle$ below the transition temperature will be uniquely aligned, $\mathbf{S}_i \parallel \mathbf{h}$. When we then send $\mathbf{h} \to 0$ in a subsequent step, that particular state will remain the observable reference state of the system. Although, formally, a spontaneous thermal fluctuation rotating all spins by the same amount $|\mathbf{S}\rangle \to |g\mathbf{S}\rangle$ would not cost energy, that flucutation can be excluded by entropic reasoning.[15] (By analogy, one rarely observes kettles crashing into the kichen wall as a consequence of a concerted thermal fluctuation of the water molecules!)

However, the appearance of non–trivial ground states is just one manifestation of spontaneous symmetry breaking. Equally important, residual fluctuations around the ground state lead to the formation of **soft modes** (sometimes known as **massless modes**), i.e. field configurations $\phi_{\mathbf{q}}$ whose action $S[\phi]$ vanishes in the limit of long wavelengths $\mathbf{q} \to 0$. Specifically, the soft modes formed on top of a symmetry broken ground state are called **Goldstone modes**. As a rule, the presence of soft modes in a continuum theory has important phenomenological consequences. To understand this point, notice that the general structure of a soft mode action is given by

$$S[\phi] = \sum_{\mathbf{q},i} \phi_{\mathbf{q}} \left[c_1^i |q_i| + c_2^i q_i^2\right] \phi_{-\mathbf{q}} + \mathcal{O}(\phi^4, q^3)\,, \tag{5.12}$$

where $c_{1,2}^i$ are coefficients. The absence of a constant contribution to the action (i.e. a contribution that does not vanish in the limit $q \to 0$) signals the existence of long–ranged power–law correlations in the system. As we will see shortly, the vanishing of the action in the long wavelength limit $q \to 0$ further implies that the contribution of the soft modes dominates practically all observable properties of the system.

5.3.3 Superfluidity

As we have seen, the theory of the weakly interacting superfluid to be discussed below was originally conceived by Bogoliubov, then in the language of second quantisation.[16] In the following, we will reformulate the theory in the language of the field integral starting

[15] Note that this (overly) simple picture in fact breaks down in dimensions $d \leq 2$, cf. our discussion of the thermal fluctuations of the ferromagnet in chapter 2.

[16] Bogoliubov, N. N., *On the Theory of Superfluidity*, J. Phys. (USSR) **11**, 23 (1947), (reprinted in D. Pines, *The Many–body Problem*, W. A. Benjamin, New York, 1961).

with the action of the weakly interacting Bose gas (5.9). Focussing on temperatures below T_c, ($\mu > 0$), let us expand the theory around the particular mean–field ground state $\bar{\psi}_0 = \psi_0 = (\mu L^d/g)^{1/2} = \gamma$. (Of course, any other state lying in the 'Mexican hat' minimum of the action would be just as good.) Notice that the quantum ground state corresponding to the configuration ψ_0 is unconventional in the sense that it cannot have a definite particle number. The reason is that, according to the correspondence $\psi \leftrightarrow a$ between coherent states and operators, respectively, a non–vanishing functional expectation value of ψ_0 is equivalent to a non–vanishing quantum expectation value $\langle a_0 \rangle$. Assuming that, at low temperatures, the thermal average $\langle \ldots \rangle$ will project onto the ground state $|\Omega\rangle$, we conclude that $\langle \Omega | a_0 | \Omega \rangle \neq 0$, i.e. $|\Omega\rangle$ cannot be a state with a definite number of particles.[17]

The symmetry group U(1) acts on this state by multiplication, $\psi_0 \to e^{i\phi}\psi_0$ and $\bar{\psi}_0 \to e^{-i\phi}\bar{\psi}_0$. Knowing that the action of a weakly modulated field $\phi(\mathbf{r}, \tau)$ will be massless, let us introduce coordinates

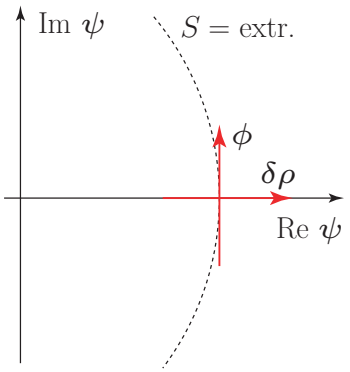


Figure 5.8: Schematic diagram showing the coordinates of the massive ($\delta\rho$) and massless ($\delta\phi$) fluctuations.

$$\psi(\mathbf{r}, \tau) = [\rho_0 + \delta\rho(\mathbf{r}, \tau)]^{1/2} e^{i\phi(\mathbf{r},\tau)},$$
$$\bar{\psi}(\mathbf{r}, \tau) = [\rho_0 + \delta\rho(\mathbf{r}, \tau)]^{1/2} e^{-i\phi(\mathbf{r},\tau)},$$

where $\rho_0 \equiv \gamma^2 = \bar{\psi}_0\psi_0$ is the condensate density. Evidently, the variable $\delta\rho$ parameterizes deviations of the field $\psi(\mathbf{r}, \tau)$ from the extremum. These excursions are energetically costly, i.e. $\delta\rho$ will turn out to be a massive mode. Also notice that the transformation of coordinates $(\bar{\psi}, \psi) \to (\delta\rho, \phi)$, viewed as a change of integration variables, has a Jacobian of unity.

▷ INFO. As we are dealing with a (functional) integral, there is a lot of freedom as to the choice of integration parameters. (I.e. in contrast to the operator formulation, there is no *a priori* constraint for a transform to be 'canonical'.) However, physically meaningful changes of representation will usually be **canonical transformations**, in the sense that the corresponding

[17] However, as usual with grand canonical descriptions, in the thermodynamic limit, the relative uncertainty in the number of particles, $(\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2)/\langle \hat{N} \rangle^2$ will become vanishingly small.

transformations of operators would conserve the commutation relations. Indeed, one may confirm that the operator transformation $a(\mathbf{r}) \equiv \hat{\rho}(\mathbf{r})^{1/2}\, e^{i\hat{\phi}(\mathbf{r})}$, $a^\dagger(\mathbf{r}) \equiv e^{-i\hat{\phi}(\mathbf{r})}\, \hat{\rho}(\mathbf{r})^{1/2}$, fulfills this criterion (exercise).

We next substitute the density–phase relation into the action and expand to second order around the reference mean–field. Ignoring gradients acting on the density field (in comparison with the 'potential' cost of these fluctuations), we obtain

$$S[\delta\rho, \phi] \approx \int d^d r \int d\tau \left[i\rho\partial_\tau\phi + \frac{\rho_0}{2m}(\partial\phi)^2 + \frac{g\delta\rho^2}{2} \right] . \tag{5.13}$$

The first term of the action has the canonical structure 'momentum $\times\, \partial_\tau$(coordinate)' indicative of a canonically conjugate pair. The second term measures the energy cost of spatially varying phase flucutations. Notice that fluctuations with $\phi(\mathbf{r}, \tau) =$ const. do not incur an energy cost — ϕ is a Goldstone mode. Finally, the third term records the energy cost of massive fluctuations from the potential minimum. Eq. (5.13) represents the Hamiltonian version of the action, i.e. an action comprising coordinates ϕ and momenta $\delta\rho$. Gaussian integration over the field $\delta\rho$ leads us to the Lagrangian form of the action (exercise):

$$S[\phi] \approx \frac{1}{2} \int d^d r \int d\tau \left[\frac{1}{g}(\partial_\tau\phi)^2 + \frac{\rho_0}{m}(\partial\phi)^2 \right] . \tag{5.14}$$

Comparison with Eq. (1.2) identifies this action as the familiar the d–dimensional oscillator. Drawing on the results of chapter 1 (see, e.g., Eq. (1.15)), we find that the energy $\omega_{\mathbf{k}}$ carried by elementary excitations of the system scales linearly with momentum, $\omega_{\mathbf{k}} = |\mathbf{k}|\rho_0/mg$.

Let us now discuss the physical ramifications of these results. The actions (5.13) and (5.14) describe the phenomenon of superfluidity. To make the connection between the fundamental degree of freedom of a superfluid system, the **supercurrent**, and the phase field explicit, let us consider the quantum mechanical current operator

$$\begin{aligned} \hat{\mathbf{j}}(\mathbf{r}, \tau) &= \frac{i}{2m} \left[(\nabla a^\dagger(\mathbf{r}, \tau)) a(\mathbf{r}, \tau) - a^\dagger(\mathbf{r}, \tau) \nabla a(\mathbf{r}, \tau) \right] \overset{\text{fun. int}}{\longrightarrow} \\ &\to \frac{i}{2m} \left[(\nabla\bar{\psi}(\mathbf{r}, \tau))\psi(\mathbf{r}, \tau) - \bar{\psi}(\mathbf{r}, \tau)\nabla\psi(\mathbf{r}, \tau) \right] \approx \frac{\rho_0}{m}\nabla\phi(\mathbf{r}, \tau), \end{aligned} \tag{5.15}$$

where the arrow indicates the functional integral correspondence of the operator description and we have neglected all contributions arising from spatial fluctuations of the density profile. (Indeed, these — massive — fluctuations describe the 'normal' contribution to the current flow.)

▷ Info. **Superfluidity** is one of the most counterintuitive and fascinating phenomena displayed by condensed matter systems. Experimentally, the most straightforward access to superfluid states of matter is provided by the Helium liquids. Representative of many other effects displayed by superfluid states of Helium, we mention the capability of thin films to flow up the walls of a vessel (if the reward is that on the outer side of the container a low lying basin can be reached — the fountain experiment) or to effortlessly propagate through porous media

that no normal fluid may penetrate.

The gradient of the phase variable is therefore a measure of the (super)current flow in the system. The behaviour of that degree of freedom can be understood by inspection of the stationary phase equations — alias, the Hamilton or Lagrange equations of motion — associated with the actions (5.13) or (5.14). Turning to the Hamiltonian formulation, one obtains (exercise)

$$i\partial_\tau \phi = -g\delta\rho, \qquad i\partial_\tau \delta\rho = \frac{\rho_0}{m}\partial^2\phi = \nabla\cdot\mathbf{j}.$$

The second of these equations represents (the Euclidean time version) of a continuity equation. A current flow with non–vanishing divergence is accompanied by dynamical distortions in the density profile. The first equation tells us that the system adjusts to spatial fluctuations of the density by a dynamical phase fluctuation. The most remarkable feature of these equations is that they possess steady state solutions with non–vanishing current flow. Setting $\partial_\tau\phi = \partial_\tau\delta\rho = 0$, we obtain the conditions $\delta\rho = 0$ and $\nabla\cdot\mathbf{j} = 0$, i.e. below the condensation temperature, a configuration with a uniform density profile can support a steady state divergenceless (super)current. Notice that a 'mass term' in the ϕ action would spoil this property, i.e. within our present approach, the phenomenon of supercurrent flow is intimately linked to the Goldstone mode character of the ϕ field.

▷ EXERCISE. Add a ficticious mass term to the ϕ–action (viz. $\delta\mathcal{L} = m\phi^2$) and explore its consequences. How do the features discussed above present themselves in the Lagrange picture?

It is very instructive to interpret the phenomenology of supercurrent flow from a different, more microscopic perspective. Steady state current flow in normal environments is prevented by the mechanism of **energy dissipation**, i.e. particles constituting the current flow scatter off imperfections inside the system thereby converting part of their energy into the creation of elementary excitations. (Macroscopically, the conversion of kinetic energy into the creation of excitations manifests itself as heat production.) Apparently, this mechanism is inactivated in superfluid states of matter, i.e. the current flow is dissipationless.

How can the dissipative loss of energy be avoided. Trivially, no energy can be exchanged if there are no elementary excitations to create. In reality, this means that the excitations of the system are energetically high–lying such that the kinetic energy stored in the current–carrying particles is insufficient to create them. But this is not the situtation that we encounter in the superfluid! As we saw above, there is no energy gap separating the quasi–particle excitations of the system from the ground state. Rather, the dispersion $\omega(\mathbf{k})$ vanishes linearly as $\mathbf{k} \to 0$. However, there is an ingenuous argument due to Landau showing that a linear excitation spectrum indeed suffices to stabilize dissipationless transport:

▷ INFO. Consider the flow of some fluid through a pipe (cf. Fig. 5.9 top left). To be concrete, let us assume that the flow occurs at a uniform velocity $\mathbf{V}$. Taking the mass (of a certain portion of the fluid) to be M, the current carries a total kinetic energy $E_1 = M\mathbf{V}^2/2$. Now, suppose we view the situation from the point of view of the fluid, i.e. we perform a Galileian transformation

into its own rest frame (see Fig. 5.9, top right). From the perspective of the fluid, the walls of the pipe appear as though they were moving with velocity $-\mathbf{V}$. Now, suppose that frictional forces between fluid and the wall lead to the creation of an elementary excitation of momentum $\mathbf{p}$ and energy $\epsilon(\mathbf{p})$, i.e. the fluid is no longer at rest but carries kinetic energy. After a Galileian transformation back to the laboratory frame, one finds that the energy of the fluid after the creation of the excitation is given by (excercise)

$$E_2 = \frac{M\mathbf{V}^2}{2} + \mathbf{p}\cdot\mathbf{V} + \epsilon(\mathbf{p})\,.$$

Now, since all of the energy needed to manufacture the excitation must have been provided by

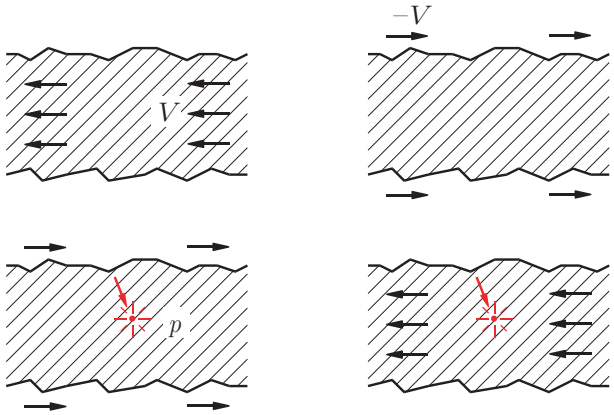


Figure 5.9: Top left: Flow of a fluid through a rough pipe. Top right: The same viewed from the rest frame of the fluid. Bottom left: Dissipative creation of a (quasi–particle) excitation. Bottom right: The same viewed from the laboratory frame.

the liquid itself, energy conservation requires that $E_1 = E_2$, or $-\mathbf{p}\cdot\mathbf{V} = \epsilon(\mathbf{p})$. Since $\mathbf{p}\cdot\mathbf{V} > -|\mathbf{p}||\mathbf{V}|$, this condition can only be met if $|\mathbf{p}||\mathbf{V}| > \epsilon(\mathbf{p})$. While systems with a 'normal' gapless dispersion, $\epsilon(\mathbf{p}) \sim \mathbf{p}^2$ are compatible with this energy–balance relation (i.e. no matter how small $|\mathbf{V}|$, quasi–particles of low momentum can always be excited), both gapped dispersions $\epsilon(\mathbf{p}) \stackrel{\mathbf{p}\to 0}{\longrightarrow}$ const. and linear dispersions are incompatible if $\mathbf{V}$ becomes smaller than a certain **critical velocity** V_*. Specifically for a linear dispersion $\epsilon(\mathbf{p}) = v|\mathbf{p}|$, the critical velocity is given by $V_* = v$. For currents slower than that, the flow is necessarily dissipationless.

Let us conclude our preliminary discussion of the weakly interacting Bose gas with a very important remark. Superficially, Eqs. (5.13) and (5.14) suggest that we have managed to describe the long–range behaviour of the condensed matter system in terms of a free Gaussian theory. However, one must recall that ϕ is a phase field, defined only modulo 2π. (In Eqs. (5.13) and (5.14) this condition is understood implicitly. At this point, it is perhaps worth reiterating that when dealing with Goldstone modes it is important to keep the underlying geometry in mind and not too tightly focus on a specific coordinate representation.) The fact that ϕ is defined only up to integer multiples of 2π manifests itself in the formation of the most interesting excitations of the superfluid; **vortices**, i.e. phase configurations $\phi(\mathbf{r},\tau)$ that change by a multiple of 2π as one moves around a certain reference coordinate, the vortex centre. Existing in parallel with harmonic phonon–like

excitations discussed above, these excitations lead to a wealth of observable phenomena. However, leaving such effects aside, let us turn to the discussion of another prominent superfluid, the condensate of Cooper pairs, more generally known as the superconductor.

5.4 Superconductivity

The electrical resistivity of many metals and alloys drops suddenly to zero when the specimen is cooled to a sufficiently low temperature. This phenomenon, which goes by the name **superconductivity**, was first observed by Kammerlingh Onnes in Leiden in 1911, three years after he first liquefied Helium.[18] Perhaps more striking, a superconductor cooled below its transition temperature in a magnetic field expels all magnetic flux from its interior. This phenomenon of *perfect diamagnetism* is known as the **Meissner effect** and is characteristic of superconductivity.

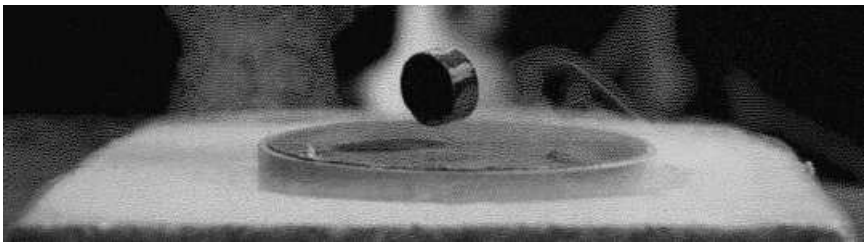
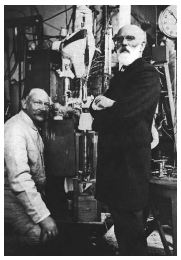


Figure 5.10: The levitation of a magnet above a (high temperature) superconductor due to the expulsion of magnetic flux.

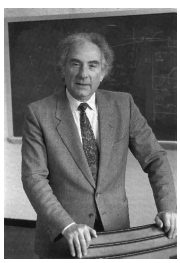
The superconducting state is an ordered state of the conduction electrons of the metal. The nature and origin of the ordering was explained by Bardeen, Cooper and Schrieffer.[19] At low temperatures, the presence of an attractive pairwise interaction can induce an instability of the electron gas towards the formation of bound pairs of time-reversed states

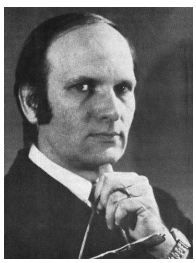
[18]



Kammerlingh Onnes 1853-1926 (left, photographed with van der Waals): 1913 Nobel Laureate in Physics for his investigations on the properties of matter at low temperatures which led, *inter alia* to the production of liquid helium.

[19] J. Bardeen, L. N. Cooper and J. R. Schrieffer, Phys. Rev. **106**, 162 (1957); **108**, 1175 (1957).





John Bardeen 1908-1991 (left), Leon N. Cooper 1930- (centre), and J. Robert Schrieffer 1931- (right): 1972 Nobel Laureate in Physics for their jointly developed theory of superconductivity. (Bardeen was also recipient of the 1956 Nobel Laureate in Physics for his research on semiconductors and discovery of the transistor effect.

$\mathbf{k}\uparrow$ and $-\mathbf{k}\downarrow$ in the vicinity of the Fermi surface. We have already seen (in section 2.2.6) how the exchange of lattice vibrations or phonons can induce an attractive interaction of electrons within the Debye frequency ω_D of the Fermi surface. Being made up of two electrons, these *composite objects*, known as **Cooper pairs** behave as bosons. At low temperatures, these bosonic degrees of freedom form a condensate which is responsible for the remarkable properties of superconductors such as perfect diamagnetism.

To explore the phenomenology of the Cooper instability of the electron gas, we will adopt a simplified model known as the pairing or reduced Hamiltonian

$$\boxed{\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} - g \sum_{kk'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}}$$

Although, strictly speaking, a realistic model of attraction would involve a more complicated momentum-dependent interaction such as the one obtained from the consideration of the electron-phonon interaction in section 2.2.6, the simple pairing interaction captures the essential physics. More importantly, to simplify our discussion, we will take the electrons to be otherwise non-interacting. In fact, the presence of a repulsive Coulomb interaction of the electrons plays a crucial role in the controlling properties of the superconductor, a point to which we will return later.

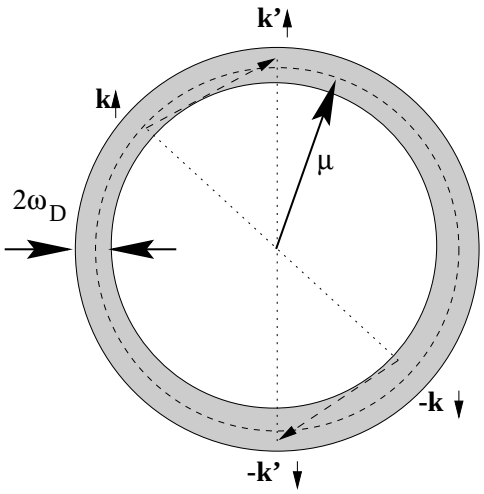


Figure 5.11: Schematic diagram showing the Fermi surface of the electron gas. The attractive interaction mediated by the exchange of phonons allows electrons within the Debye frequency ω_D of the Fermi surface to pair.

Before turning to the field theoretic formulation, we will begin by investigating a mean-field theory of the BCS transition from the stand point of the second quantisation.

5.4.1 Mean-Field Theory of Superconductivity

In its present form, the Hamiltonian explicitly involves a two-body interaction of the electrons. As such, it seems infeasible to develop an exact many-body treatment of the

Hamiltonian. Instead we will seek an approximation which renders the Hamiltonian bilinear in the electron operators and, therefore, tractable. As usual in physics, our method relies on the expected structure of the ground state wavefunction. In particular, anticipating that electrons in time-reversed states pair, let us suppose that

$$\Delta = g\sum_{\mathbf{k}}\langle \text{g.s.}|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|\text{g.s.}\rangle, \qquad \Delta^* = g\sum_{\mathbf{k}}\langle \text{g.s.}|c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}|\text{g.s.}\rangle$$

acquires a non-zero expectation value in the ground state. Here Δ represents an **order parameter** becoming non-zero in the condensed phase and therefore signalling the transition to the superconducting state. At first sight, a non-zero expectation value Δ looks strange: such a result would imply that the ground state wavefunction of the superconducting condensate is not an eigenstate of particle number (while one can see that the Hamiltonian commutes with $\hat{N}$). However, later, we will see that in the grand canonical ensemble the ground state wavefunction is a superposition of states involving many particles but strongly peaked around the thermodynamic density N/L^d.

To develop the mean-field approximation, let us set

$$g\sum_{\mathbf{k}} c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} = \Delta + \overbrace{\left(g\sum_{\mathbf{k}} c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} - \Delta\right)}^{\text{small}}$$

and keep only terms which depend up to quadratic order in the electron operators. Adding the chemical potential, the 'mean-field' Hamiltonian takes the form

$$\hat{H} - \mu\hat{N} \simeq \sum_{\mathbf{k}}\Big[\sum_{\sigma}\overbrace{(\epsilon_{\mathbf{k}}-\mu)}^{\xi_{\mathbf{k}}} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} - \left(\Delta^* c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} + \Delta c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\right)\Big] + \frac{|\Delta|^2}{g}$$

known as the **Bogoluibov** or **Gor'kov** Hamiltonian. In this simplified form, it is interesting to note that the Hamiltonian does not now conserve particle number. Instead, pairs of particles are born and annihilated out of the vacuum.

To bring the mean-field Hamiltonian to a diagonal form, it is convenient to recast it in a **Nambu spinor** representation defining

$$\Psi^\dagger_{\mathbf{k}} = \begin{pmatrix} c^\dagger_{\mathbf{k}\uparrow} & c_{-\mathbf{k}\downarrow}\end{pmatrix}, \qquad \Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow}\end{pmatrix}$$

after which the Hamiltonian takes the form (exercise: recall the fermionic anticommutation relations of the electron operators)

$$\boxed{\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}}\left[\Psi^\dagger_{\mathbf{k}}\begin{pmatrix}\xi_{\mathbf{k}} & -\Delta \\ -\Delta^* & -\xi_{\mathbf{k}}\end{pmatrix}\Psi_{\mathbf{k}} + \xi_{\mathbf{k}}\right] + \frac{|\Delta|^2}{g}}$$

Now, being bilinear in the electron operators, the mean-field Hamiltonian can be brought to a diagonal form by employing the unitary transformation

$$\chi^\dagger_{\mathbf{k}} \equiv \begin{pmatrix}\alpha^\dagger_{\mathbf{k}\uparrow} \\ \alpha_{-\mathbf{k}\downarrow}\end{pmatrix} = \begin{pmatrix}\cos\theta_{\mathbf{k}} & \sin\theta_{\mathbf{k}} \\ \sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}c^\dagger_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}\end{pmatrix} \equiv U\psi^\dagger_{\mathbf{k}},$$

(under which the anticommutation relations of the new electron operators $\alpha_{\mathbf{k}\sigma}$ are maintained: exercise). Note that the notation is purely symbolic: $\alpha^\dagger_{\mathbf{k}\uparrow}$ involves a superposition of $c^\dagger_{\mathbf{k}\uparrow}$ and $c_{-\mathbf{k}\downarrow}$. Choosing Δ to be real,[20] and setting $\tan(2\theta_{\mathbf{k}}) = -\Delta/\xi_{\mathbf{k}}$, i.e. $\cos(2\theta_{\mathbf{k}}) = \xi_{\mathbf{k}}/\lambda_{\mathbf{k}}$, $\sin(2\theta_{\mathbf{k}}) = -\Delta/\lambda_{\mathbf{k}}$, where $\lambda_{\mathbf{k}} = (\Delta^2 + \xi^2_{\mathbf{k}})^{1/2}$, the transformed Hamiltonian takes the form (exercise)

$$\begin{aligned}\hat{H} - \mu\hat{N} &= \sum_{\mathbf{k}} \lambda_{\mathbf{k}} \left(\alpha^\dagger_{\mathbf{k}\uparrow}\alpha_{\mathbf{k}\uparrow} - \alpha_{-\mathbf{k}\downarrow}\alpha^\dagger_{-\mathbf{k}\downarrow} \right) + \sum_{\mathbf{k}} \xi_{\mathbf{k}} + \frac{\Delta^2}{g} \\ &= \sum_{\mathbf{k}\sigma} \lambda_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - \lambda_{\mathbf{k}}) + \frac{\Delta^2}{g}\end{aligned}$$

This result shows that the elementary excitations or quasi-particle states, known as "**Bogoluibons**", created by $\alpha^\dagger_{\mathbf{k}\sigma}$, have a minimum energy Δ, the energy gap.

To determine the ground state wavefunction one simply has to identify the state which is annihilated by all the quasi-particle annihilation operators $\alpha_{\mathbf{k}\sigma}$. This condition is met uniquely by the state

$$\boxed{|\text{g.s.}\rangle = \prod_{\mathbf{k}} \alpha_{\mathbf{k}\uparrow}\alpha_{-\mathbf{k}\downarrow}|\Omega\rangle \propto \prod_{\mathbf{k}} \left(\cos\theta_{\mathbf{k}} - \sin\theta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right) |\Omega\rangle}$$

where $|\Omega\rangle$ represents the vacuum state, and

$$2\sin^2\theta_{\mathbf{k}} = 1 - \frac{\xi_{\mathbf{k}}}{\lambda_{\mathbf{k}}}$$

Physically, in the limit $\Delta \to 0$, $\sin^2\theta_{\mathbf{k}} \to \theta(\mu - \epsilon_{\mathbf{k}})$, and the ground state collapses to the filled Fermi sea with chemical potential μ. As Δ becomes non-zero, states in the vicinity of the Fermi surface rearrange themselves into a bound state condensate and lower their energy.

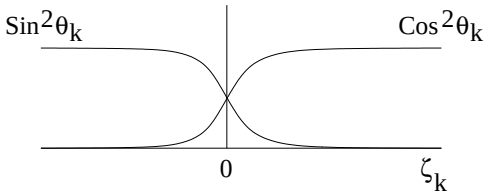


Figure 5.12: Schematic diagram showing the variation of the occupancy of the momemtum basis states in the ground state; $\sin^2\theta_k$ represents the occupancy of the $\mathbf{k}$ states. Note that the wavefunction of the ground state condensate involves the occupation of basis states with momentum in excess of $p_F = \sqrt{2m\mu}$.

An estimate of the corresponding ground state energy obtains

$$E_{\text{g.s.}} \equiv \langle \text{g.s.}|\hat{H} - \mu\hat{N}|\text{g.s.}\rangle = \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - \lambda_{\mathbf{k}}) + \frac{\Delta^2}{g},$$

[20] One may show that the phase of Δ may be chosen arbitrarily, a fact to which we will return later.

a result which always lowers the energy below the non-interacting $g = 0$ theory (exercise).

Finally, to determine the scale of the order parameter we have to determine self-consistently the order parameter, viz.,

$$\begin{aligned}\Delta &= g\sum_{\mathbf{k}}\langle \text{g.s.}|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|\text{g.s.}\rangle = -g\sum_{\mathbf{k}}\sin\theta_{\mathbf{k}}\cos\theta_{\mathbf{k}} \\ &= \frac{g}{2}\sum_{\mathbf{k}}\frac{\Delta}{(\Delta^2+\xi_{\mathbf{k}}^2)^{1/2}} \simeq \frac{gL^3\Delta}{2}\nu(\mu)\int_{-\omega_D}^{\omega_D}\frac{d\xi}{(\Delta^2+\xi^2)^{1/2}} = gL^3\Delta\nu(\mu)\sinh^{-1}(\omega_D/\Delta)\end{aligned}$$

where $\sum_{\mathbf{k}} \to \int d\xi\ \nu(\xi)$ and $\nu(\xi)$ denotes the density of states. (It is left as an exercise to show that a minimisation of the g.s. energy obtains the same self-consistent equation for the order parameter.) Here we have assumed that the pairing interaction g extends over an energy scale set by ω_D. Physically, for pairing mechanisms which derive from the exchange of phonons, this energy scale is set by the corresponding Debye frequency, the maximum energy phonon. Finally rearranging this equation, one obtains

$$\boxed{\Delta = \frac{\omega_D}{\sinh(1/gL^3\nu(\mu))} \simeq 2\omega_D\exp\left[-\frac{1}{gL^3\nu(\mu)}\right]}$$

This completes our formal investigation of the BCS transition from the mean-field Hamiltonian. How does the same transition emerge from the corresponding field theory? In the following, we will develop a theory of superconductivity from the coherent state path integral for the quantum partition function.

5.4.2 Superconductivity from the Path Integral

To investigate the BCS transition within the framework of the coherent state path integral, it is convenient to abandon the long-ranged pairing Hamiltonian considered above and introduce a space-local attractive interaction contained within the **BCS Hamiltonian**,

$$\hat{H}_{\text{BCS}} = \int d^dr\left[\sum_\sigma c_\sigma^\dagger(\mathbf{r})\frac{\hat{\mathbf{p}}^2}{2m}c_\sigma(\mathbf{r}) - gc_\uparrow^\dagger(\mathbf{r})c_\downarrow^\dagger(\mathbf{r})c_\downarrow(\mathbf{r})c_\uparrow(\mathbf{r})\right].$$

Expressed in the form of the coherent state path integral, the corresponding quantum partition function takes the form

$$\mathcal{Z} = \int_{\text{a.p.b.c.}} D(\bar{\psi},\psi)\exp\left\{-\int_0^\beta d\tau\int d^dr\left[\sum_\sigma\bar{\psi}_\sigma\left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu\right)\psi_\sigma - g\bar{\psi}_\uparrow\bar{\psi}_\downarrow\psi_\downarrow\psi_\uparrow\right]\right\},$$

where $\psi(\mathbf{r},\tau)$ represent anticommuting or Grassmann fields and the nemonic a.p.b.c. denotes anti-periodic boundary conditions. As usual the quartic interaction of the fields prevents the partition function from being evaluated explicitly. Moreover, anticipating the existence of a transition of the electron gas to a condensed phase in which electrons in the vicinity of the Fermi surface are paired, we can expect that a perturbative expansion in the coupling constant g will be inadequate. Motivated by the mean-field theory discussed

above, we will instead introduce a bosonic field Δ to decouple the interaction and which will have the physical significance of the complex order parameter.

The decoupling is arranged using a **Hubbard-Stratonovich** transformation

$$e^{g\int d\tau \int d^dr \bar\psi_\uparrow \bar\psi_\downarrow \psi_\downarrow \psi_\uparrow} = \int D(\Delta^*,\Delta) \exp\left\{ -\int d\tau \int d^dr \left[\frac{1}{g}|\Delta|^2 - \left(\Delta^* \psi_\downarrow \psi_\uparrow + \Delta \bar\psi_\uparrow \bar\psi_\downarrow \right) \right] \right\}$$

where $\Delta(\mathbf{r},\tau)$ represents a dynamically fluctuating **bosonic** or complex field with a symmetry that reflects that of the bilinear $\psi_\downarrow\psi_\uparrow$. Taking Δ to be homogeneous in space and time, the quantum Hamiltonian corresponding to the action coincides with that of the mean-field Hamiltonian considered in the previous section. Motivated by that analysis, we turn to the **Nambu spinor** representation

$$\bar\Psi = \begin{pmatrix} \bar\psi_\uparrow & \psi_\downarrow \end{pmatrix}, \qquad \Psi = \begin{pmatrix} \psi_\uparrow \\ \bar\psi_\downarrow \end{pmatrix}.$$

wherein the quantum partition function assumes the form

$$\begin{aligned} \mathcal{Z} &= \int D(\bar\psi,\psi) \int D(\Delta^*,\Delta) \exp\left\{ -\int d\tau \int d^dr \left[\frac{1}{g}|\Delta|^2 + \bar\Psi \hat{\mathcal{G}}^{-1} \Psi \right] \right\}, \\ \hat{\mathcal{G}}^{-1} &= \begin{pmatrix} [\hat G_0^{(\mathrm{p})}]^{-1} & -\Delta \\ -\Delta^* & [\hat G_0^{(\mathrm{h})}]^{-1} \end{pmatrix}, \end{aligned}$$

where $[\hat G_0^{(\mathrm{p})}]^{-1} = \partial_\tau + (\epsilon_{\hat{\mathbf{p}}} - \mu)$ and $[\hat G_0^{(\mathrm{h})}]^{-1} = \partial_\tau - (\epsilon_{\hat{\mathbf{p}}} - \mu)$ represents the non-interacting Green function of the particle and hole respectively, and $\hat{\mathcal{G}}$ is known as the **Gor'kov Green function**.

Being Gaussian in the fermionic fields, the functional integral over the Grassmann fields can be performed straightforwardly, and yields the formal expression

$$\mathcal{Z} = \int D(\Delta^*,\Delta) \exp\left[-\int d\tau \int d^dr \frac{1}{g}|\Delta|^2 + \ln\det \hat{\mathcal{G}}^{-1} \right],$$

where we have written $\det \mathcal{G}^{-1} = \exp[\ln\det \mathcal{G}^{-1}]$. By introducing a Hubbard-Stratonovich decoupling of the local interaction, we have succeeded in expressing the quantum partition function as a path integral over an auxiliary bosonic field Δ. Further progress is possible only within some approximation. Empirically, we know that the superconducting transition is *second order*, i.e. the order parameter Δ develops a non-zero expectation value below a critical temperature T_c growing *continuously from zero*. At temperatures $T \ll T_c$, spatial and temporal fluctuations around the expectation value $\bar\Delta$ can be treated as small. In this limit, the action can be treated within a **mean-field** approximation where the partition function is dominated by the **saddle-point configuration** of $\bar\Delta$. The saddle-point analysis, which leads to a self-consistent equation for $\bar\Delta$ known as the **Gap Equation**, is left as an exercise in Problem Set 4. Instead we will focus on temperatures $T \sim T_c$ in which an effective action for Δ can be obtained.

In the vicinity of the transition temperature T_c, the order parameter Δ is expected to be small. We are therefore at liberty to look for a perturbative expansion in powers of Δ. Setting

$$\hat{\mathcal{G}}^{-1} = \hat{\mathcal{G}}_0^{-1} \left[1 - \hat{\mathcal{G}}_0 \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix} \right],$$

where, by definition, $\hat{\mathcal{G}}_0 \equiv \hat{\mathcal{G}}(\Delta = 0)$, and expanding the action to second order in Δ,[21] the quantum partition function takes the form (exercise)

$$\mathcal{Z} = \mathcal{Z}_0 \int D(\Delta^*, \Delta) e^{-S}, \qquad S = \sum_{\omega_n, \mathbf{q}} \left[\frac{1}{g} + \Pi(\omega_n, \mathbf{q}) \right] |\Delta_{\omega_n, \mathbf{q}}|^2 + O(\Delta^4), \tag{5.16}$$

with (see Fig. 5.13a)

$$\Pi(\omega_m, \mathbf{q}) = \frac{1}{\beta L^d} \sum_{\omega_n, \mathbf{k}} G_0^{(\mathrm{p})}(\omega_n, \mathbf{k}) G_0^{(\mathrm{h})}(\omega_n + \omega_m, \mathbf{k} + \mathbf{q}).$$

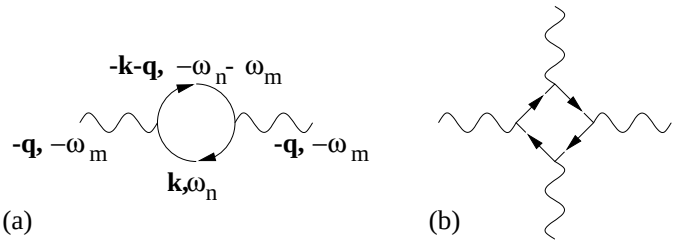


Figure 5.13: Diagrammatic representation of (a) the response function $\Pi(\omega_m, \mathbf{q})$, and (b) the quartic vertex.

An instability of the electron gas towards the formation of a paired condensate is signalled by the appearance of a non-zero expectation value of the anomalous average $\langle \psi_\uparrow \psi_\downarrow \rangle$ (i.e. $\bar{\Delta} \neq 0$). Moreover, intuitively, we would expect the action to be minimised by a spatially and temporally uniform field configuration of Δ. Applying this *Ansatz*, we are led to consider a gradient expansion of the action in powers of Δ.

Neglecting temporal fluctuations altogether, a gradient expansion in powers of $\mathbf{q}$ obtains

$$\Pi(\omega_m, \mathbf{q}) = \Pi(0,0) + \frac{1}{2}\mathbf{q}^2 \overbrace{\partial_{|\mathbf{q}|}\Pi(0,0)}^{K>0} + O(i\omega_m, \mathbf{q}^4),$$

where, by symmetry, we have made use of the fact that $\Pi = \Pi(\mathbf{q}^2)$. Substituting this expansion into Eq. (5.16), and returning to the real space representation, we obtain the static effective action

$$\boxed{S[\Delta] = \beta \int d^d r \left[\frac{t}{2} |\Delta|^2 + \frac{K}{2} |\partial \Delta|^2 + u |\Delta|^4 + \cdots \right]} \tag{5.17}$$

where $t/2 = g + \Pi(0,0)$ represents an effective 'chemical potential' for Δ, and $u > 0$ represents the constant coefficient associated with the quartic vertex (see Fig. 5.13b). (The calculation of the coefficients K and u is left as an exercise in Matsubara frequency summations! However, in the following, we will not need to know their form explicitly.)

[21] Here we have made use of the identity $\ln \det \hat{\mathcal{G}}^{-1} = \mathrm{tr} \ln \hat{\mathcal{G}}^{-1}$ to form the expansion

$$\mathrm{tr} \ln \hat{\mathcal{G}}^{-1} = \mathrm{tr} \ln \hat{\mathcal{G}}_0^{-1} + \sum_{n=1}^{\infty} \frac{1}{n} \mathrm{tr} \left[\hat{\mathcal{G}}_0 \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix} \right]^n$$

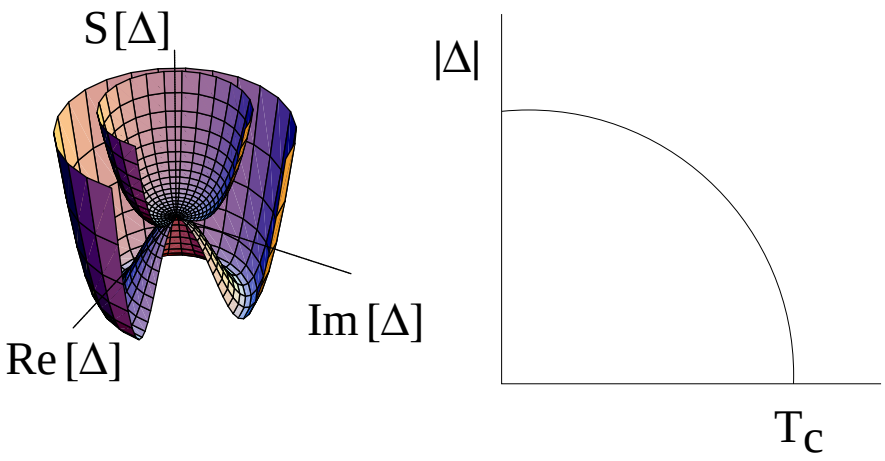


Figure 5.14: Dependence of the effective action S_0 on the complex mean-field order parameter Δ. At $t > 0$, fluctuations of Δ are energetically unfavourable whilst for $t < 0$, the action becomes unstable towards the formation of a non-zero expectation value of Δ. Also shown is the expectation value $\bar{\Delta}$ of the order parameter as a function of temperature.

5.4.3 Gap Equation

Applying a **mean-field approximation**, i.e. focusing on the spatially homogeneous component Δ_0, the effective action takes the form

$$\boxed{\frac{S[\Delta_0]}{\beta L^d} = \frac{t}{2}|\Delta_0|^2 + u|\Delta_0|^4.} \tag{5.18}$$

In particular, when the effective chemical potential t becomes negative, the expectation value of $\langle\Delta_0\rangle$ becomes finite (see Fig. 5.14). Summing over momenta, and making use of the identity $\frac{1}{L^d}\sum_{\mathbf{k}} = \int_{-\infty}^{\infty} d\xi \nu(\xi)$ where, as usual, $\nu(\xi)$ denotes the density of states at energy ξ, one obtains

$$\Pi(0,0) = -\frac{1}{\beta L^d}\sum_{\omega_n,\mathbf{k}} \frac{1}{\omega_n^2 + (\epsilon_{\mathbf{k}} - \mu)^2} \simeq -\frac{1}{\beta}\sum_{\omega_n}\int_{-\infty}^{\infty} d\xi \frac{\nu(\xi+\mu)}{\omega_n^2 + \xi^2} \simeq -\sum_{\omega_n}\frac{\pi\nu(\mu)}{\beta\omega_n}.$$

Recalling that the attractive interaction of the electrons was mediated by the exchange of phonons, we note that the Matsubara summation should be cut-off at the scale of the Debye frequency. Setting $\omega_D = (2n_{\max}+1)\pi/\beta$, we obtain

$$\Pi(0,0) \simeq -\nu(\mu)\sum_{n=-n_{\max}}^{n_{\max}} \frac{1}{2n+1} \simeq -2\nu(\mu)\int_0^{n_{\max}} \frac{dn}{2n+1} \simeq -\nu(\mu)\ln(\beta\omega_D).$$

Equating this result with $1/g$, we deduce that the electron gas becomes unstable towards the formation of a pair condensate when

$$\boxed{T < T_c \equiv \omega_D \exp\left[-\frac{1}{\nu(\mu)g}\right]}$$

Substituting this result into the expression for t we find that, in the vicinity of T_c,

$$t = 2\nu(\mu) \ln\left(\frac{T}{T_c}\right) \simeq 2\nu(\mu)\left(\frac{T-T_c}{T_c}\right),$$

i.e. one may think of the parameter t as a '**reduced temperature**'.

Finally, taking the partition function to be dominated by the minimum of the mean-field action (5.18) $\mathcal{Z} \sim \exp[-S_0(|\bar{\Delta}|)]$ (i.e. applying a saddle-point approximation), we find a spontaneous breaking of the $U(1)$ symmetry of the complex order parameter — i.e. $\bar{\Delta}$ has a magnitude (see Fig. 5.14b),

$$|\bar{\Delta}| = \begin{cases} 0 & t > 0, \\ \sqrt{t/4u} & t < 0. \end{cases}$$

with arbitrary but constant phase. This situation is reminiscent of the Heisenberg ferromagnet: the complex order parameter is isomorphic to a 'two-component' spin where the phase degree of freedom is mirrored in the orientation of the moment. According to the Mermin-Wagner theorem, the breaking of the continuous $U(1)$ symmetry should be accompanied by the appearance of massless **Goldstone modes**. The stability of the mean-field solution towards fluctuations is governed by the effective action $S[\Delta]$ (5.17).

To summarise, the quantum partition function of an electron gas subject to a local attractive pairing interaction has been cast in the form of a quantum field theory involving a complex scalar field $\Delta(\mathbf{r}, \tau)$ whose expectation value is connected to the anomalous average $\langle \psi_\uparrow \psi_\downarrow \rangle$. A gradient expansion of the effective action in powers Δ reveals an instability of the electron gas towards the formation of a spatially and temporally uniform pair condensate. Fluctuations of the order parameter Δ around its mean-field expectation value are described by a low energy effective action (5.17).

In fact, interpreted as an effective Free energy, this result might have been guessed on purely phenomenological grounds: indeed, identifying the anomalous average as an appropriate **order parameter**, Δ Eq. (5.17) is consistent with a gradient expansion of the Free energy (in powers of Δ) compatible with symmetry and the observed temperature dependences. The phenomenology of superconductivity (expressed by the free energy of (5.17) and known as the **Ginzburg-Landau Theory**) anticipated the microscopic theory of BCS.

5.4.4 †Superconductivity: Anderson-Higgs Mechanism

▷ INFO. So far, our analysis of the quantum partition function associated with the BCS Hamiltonian is incomplete. Indeed, no reference has yet been made to the characteristic or defining properties: superconductivity, and perfect diamagnetism. To discover such phenomena within our theory we have to generalise our approach to accommodate an electromagnetic field. At the microscopic level, we can do so by incorporating into the BCS Hamiltonian the canonical momentum $\mathbf{p} \to \mathbf{p} - e\mathbf{A}/c$, and introducing the classical action associated with the electromagnetic field: $\mathcal{L} = -F_{\mu\nu}F^{\mu\nu}/4$, where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ represents the electromagnetic field tensor. Leaving the formal derivation as an exercise, we can, in the spirit of Ginzburg-Landau theory,

guess the appropriate form of the resulting (time-independent) action:

$$\boxed{S = \beta \int d^d r \left[\frac{t}{2}|\Delta|^2 + \frac{K}{2}|(\partial + i2e\mathbf{A}/c)\Delta|^2 + u|\Delta|^4 + \frac{1}{2}(\partial \times \mathbf{A})^2 \right]} \tag{5.19}$$

This result can be inferred from gauge invariance of the order parameter under the local $U(1)$ transformation $\psi \to e^{ie\phi(\mathbf{r})/c}\psi$, $\Delta(\mathbf{r}) \to e^{2ie\phi(\mathbf{r})/c}\Delta(\mathbf{r})$ — see below — (or indeed obtained from first principles by generalising the derivation presented above). The apparent 'doubling of the electric charge' can be interpreted as reflecting the effective charge of a Cooper pair.

Gauge Invariance: In the presence of the electromagnetic field, the quantum partition function $\mathcal{Z} = \int D\mathbf{A} \int D[\Delta, \Delta^*] e^{-S}$ exhibits a gauge invariance under the transformation (exercise)

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} - \partial\phi, \qquad \Delta \mapsto \Delta' = e^{2ie\phi/c}\Delta.$$

That is, under such a transformation, the action remains invariant. Therefore, by gauge fixing $\partial\phi = \mathbf{A}$, the phase of the order parameter can be eliminated from the action and the effective action takes the form

$$S = \beta \int d^d r \left[\frac{t}{2}|\Delta|^2 + \frac{K}{2}(\partial|\Delta|)^2 - \frac{m_\nu^2}{2}\mathbf{A}^2 + u|\Delta|^4 + \frac{1}{2}(\partial \times \mathbf{A})^2 \right],$$

where $m_\nu^2 = 4e^2K|\Delta|^2/c^2$. As a result, we find that the massless phase degrees of freedom ϕ have disappeared from the action! They have been subsumed into the longitudinal mode of the vector field $\mathbf{A}$, which has itself become massive. This is an example of the celebrated **Anderson-Higgs mechanism**: below the transition temperature, the Goldstone bosons (in this case ϕ) and the gauge field (in this case the electromagnetic field — the photon) conspire to create massive excitations, and the massless excitations are unobservable.

It is instructive to interpret this result from the saddle-point or mean-field equations of the motion of the order parameter and vector potential. Minimising the effective action (5.19) with respect to spatial variations of $\bar{\Delta}$ and $\mathbf{A}$, one obtains the **Gross-Pitaevskii equations** (exercise)

$$\left[-K\left(\partial + 2ie\mathbf{A}/c\right)^2 + t + 4u|\Delta|^2 \right] \Delta = 0$$
$$\partial \times (\partial \times \mathbf{A}) \equiv \mathbf{j} - m_\nu^2 \mathbf{A}, \qquad \mathbf{j} = 2i\frac{e}{c}K(\Delta\partial\bar{\Delta} - \bar{\Delta}\partial\Delta).$$

Substituting the order parameter by its homogeneous mean field value and differentiating the second equation, one finds that $\partial \times (\partial \times \mathbf{B}) = -m_\nu^2\mathbf{B}$, from which it follows that

$$\left(\partial^2 - m_\nu^2\right)\mathbf{B} = 0,$$

where $\mathbf{B} = \partial \times \mathbf{A}$. This result, known as the first **London Equation**, admits $\mathbf{B} = 0$ as the only constant spatially uniform solution. In a uniform superconductor the magnetic field is zero — the **Meissner effect**. At the edge of the superconductor, this equation can be integrated to give $\mathbf{B} \sim e^{-m_\nu x}$ showing the field to penetrate a distance m_ν^{-1} — the **Penetration depth** — into the sample.

That these equations imply superconductivity can be inferred from the time derivative of the current $\partial_t \mathbf{j} = m_\nu^2 \mathbf{E}$, where $\mathbf{E}$ denotes an external electric field (the second London equation). If a uniform field is applied for a time t_0, a current $m_\nu^2 \mathbf{E} t_0$ builds up. This current remains even

if the electric field is subsequently switched off. This contrasts with conventional conductors where there is a relaxation of the current.

Superconductivity is destroyed by a sufficiently strong magnetic field. An estimate of the critical field can be made by studying the Gross-Pitaevskii equation

$$-K\left(\partial + 2ie\mathbf{A}/c\right)^2 \Delta(\mathbf{r}) = t\Delta(\mathbf{r})$$

This equation is formally equivalent to a Schrödinger equation describing a particle of charge $2e$ and mass $m = 1/2K$ in a uniform magnetic field. The lowest Landau level is defined by the condition $t/K = 2eB_c/c$. This defines the highest field where superconductivity can occur.

Finally, we remark that, to expel a magnetic field from a sample we require an energy of $B^2/2$ per unit volume to resist the magnetic pressure. This must be compensated by the condensation energy $S/\beta L^d$. If the threshold field is smaller than the critical field B_c (Type II) magnetic field penetrates the sample in the form of flux tubes. At low temperatures the latter arrange themselves in a hexagonal configuration known as an **Abrikosov vortex lattice**. Superconductors where the situation is opposite are known as Type I.

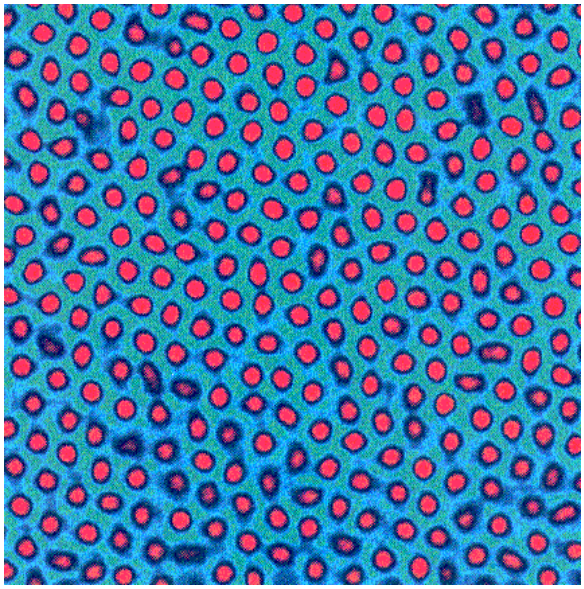


Figure 5.15: Bitter patter of an Abrikosov vortex lattice.

This concludes our formal discussion of the instability of the electron gas. For the sake of clarity we avoided a detailed discussion of the physical manifestations of the Cooper instability of the electron gas — it was used here merely as a vehicle for illustrating the general approach of the coherent state path integral. However, before leaving this section, a few remarks concerning the question of universality are in order.

5.4.5 Statistical Field Theory: Ferromagnetism Revisited

The motivation that stands behind the phenomenology of Ginzburg-Landau theory has profound implications that go beyond its application to superconductivity pervading all

areas of physics. To illustrate the generality of the concept, let us temporarily leave behind superconductivity and consider the *classical* equilibrium statistical mechanics of a 'one-component' or **Ising ferromagnet** (i.e. spin degrees of freedom can take only two values: $S_i = \pm 1$). Our previous considerations in chapter 2 have emphasised that, when viewed microscopically, the development of magnetic moments on the atomic lattice sites of a crystal and the subsequent ordering of the moments is a complex process involving the cooperative behaviour of many interacting electrons. However, at first sight, this picture seems to be at odds with the empirical observation that thermodynamic properties of different macroscopic ferromagnetic systems seem to be the same — e.g. temperature dependence of the specific heat, susceptibility, etc. Moreover, the thermodynamic critical properties of completely different physical systems, such as an Ising ferromagnet and a liquid at its boiling point, show the same dependence on, say, temperature. What is the physical origin of this **Universality**?

Suppose we take a ferromagnetic material and measure some of its material properties such as its magnetisation. Dividing the sample into two roughly equal halves, keeping the internal variables like temperature and magnetic field the same, the macroscopic properties of each piece will then be the same as the whole. The same holds true if the process is repeated. But eventually, after many iterations, something different must happen because we know that the magnet is made up of electrons and ions. The characteristic length scale at which the overall properties of the pieces begins to differ markedly from those of the original defines a **correlation length**. It is the typical length scale over which the fluctuations of the microscopic degrees of freedom are correlated.

Now experience tells us that a ferromagnet may abruptly change its macroscopic behaviour when the external conditions such as the temperature or magnetic field are varied. The points at which this happens are called **critical points**, and they mark a **phase transition** from one state to another. In the ferromagnet, there are essentially two ways in which the transition can occur (see Fig. 5.16). In the first case, the two states on either side of the critical point (spin up) and (spin down) coexist at the critical point. Such transitions, involve **discontinuous** behaviour of thermodynamic properties and are termed **first-order**. (c.f. melting of a three-dimensional solid) The correlation length at such a first-order transition is generally finite.

In the second case, the transition is **continuous**, and the correlation length becomes effectively infinite. Fluctuations become correlated over all distances, which forces the whole system to be in a unique, critical, phase. The two phases on either side of the transition (paramagnetic and ferromagnetic) must become identical as the critical point is approached. Therefore, as the correlation length diverges, the magnetisation goes smoothly to zero. The transition is said to be **second-order**.

The divergence of the correlation length in the vicinity of a second order phase transition suggests that properties near the critical point can be accurately described within an effective theory involving only long-range collective fluctuations of the system. This invites the construction of a phenomenological Hamiltonian or Free energy which is constrained only by the fundamental symmetries of the system — **Ginzburg-Landau theory**. Although the detailed manner in which the material properties and microscopic couplings of the ferromagnet influence the parameters of the effective theory might be unknown, qualitative properties such as the **scaling** behaviour are completely defined.

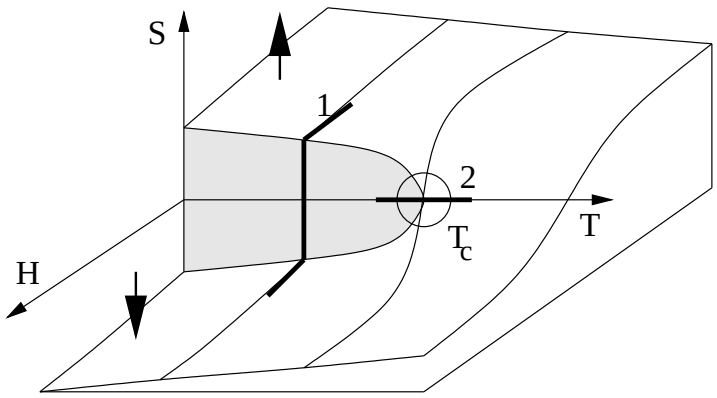


Figure 5.16: Phase diagram of the Ising ferromagnet showing the average magnetisation S as a function of magnetic field H and Temperature T. Following trajectory 1 by changing the magnetic field at constant temperature $T < T_c$, the sample undergoes a first order phase transition from an average 'spin-up' phase to an average 'spin-down'. By changing the temperature at fixed zero magnetic field, the system undergoes a second order phase transition at $T = T_c$ where the average magnetisation grows continuously from zero. This second order transition is accompanied by a *spontaneous symmetry breaking* in which the system chooses to be in either an up or down-spin phase. (Contrast this phase diagram with that of the liquid-gas transition — magnetisation $S \to$ density ρ, and magnetic field $H \to$ pressure.) The circle marks the region in the vicinity of the critical point where the correlation length is large as compared to the microscopic scales of the system, and Ginzburg-Landau theory applies.

Following this philosophy, the Ginzburg-Landau theory of the Ising ferromagnet is defined by gradient expansion of the effective Free energy in powers of the order parameter, the local magnetisation $S(\mathbf{r})$. Respecting the symmetry properties of the microscopic Hamiltonian (translational and rotational invariance in the spatial degrees of freedom, up-down or Z_2 invariance in the internal spin degrees of freedom, etc), the partition function of the Ising ferromagnet can be expressed in the form of a functional field integral over different spin configurations $S(\mathbf{r})$

$$\mathcal{Z} = \int DS(\mathbf{r}) e^{-\beta H[S(\mathbf{r})]},$$

with the effective Ginzburg-Landau Hamiltonian or Free energy functional

$$\beta H[S(\mathbf{r})] = \int d^d r \left[\frac{t}{2} S^2 + \frac{K}{2} \left(\partial S\right)^2 + uS^4 + \cdots + HS \right].$$

At the mean-field level (i.e. neglecting fluctuations of the magnetisation field) a minimisation of the effective Free energy (in the absence of an external magnetic field)

$$\frac{\beta H(S)}{V} = \frac{t}{2} S^2 + uS^4,$$

known as the **Landau Free energy**, leads to the average magnetisation

$$\bar{S} = \begin{cases} 0 & t > 0, \\ \sqrt{t/4u} & t < 0. \end{cases}$$

Thus a non-zero magnetisation develops when $t < 0$ identifying this parameter as the reduced temperature $t = (T - T_c)/T_c$.

The Ginzburg-Landau Free energy can be compared with that obtained from the microscopic Hamiltonian for the superconductor above (5.17). Apart from the complex nature of the order parameter Δ, the action coincides. In fact, we might very well have circumvented the analysis of the microscopic Hamiltonian, and written the Ginzburg-Landau Free energy on purely phenomenological grounds. The dependence of the parameters K, u, etc., on the microscopic or material properties of the system would have been unavailable, but the nature of the critical point and the physical properties associated with the transition would have been accessible. Indeed, as mentioned above much of the phenomenology of conventional superconductivity was developed and understood in this framework even prior to the discovery of the BCS theory.

From this result, we can draw important conclusions: Critical properties in the vicinity of a both classical and quantum second order phase transitions fall into a limited number of **universality classes** defined, not by detailed material parameters, but by the fundamental symmetries of the system. When we study the critical properties of the Ising transition in a one-component ferromagnet, we learn about the nature of the liquid-gas transition! Similarly, in the jargon of statistical field theory, the superconductor, with its complex order parameter Δ is in the same universality class as the two-component or XY Heisenberg ferromagnet. The analyses of critical properties associated with different universality classes is the subject of **Statistical field theory**.

1.3 Problem Set

1.3.1 Questions on Collective Modes and Field Theories

1. In obtaining the spectrum of collective phonon excitations for the lattice Lagrangian (1.1), a continuum approximation was employed. However, since the degrees of freedom are coupled linearly, the equations of motion can be solved explicitly, even for the discrete model. By constructing the equations of motion, obtain the **normal modes** of the system and obtain the exact eigenspectrum of phonon excitations. [Hint: Look for a wave-like solution of the discrete equations of motion.] Identify the limit in which the spectrum of the discrete lattice model coincides with that obtained for the continuum approximation of the model. In what limit does the continuum approximation fail and why?

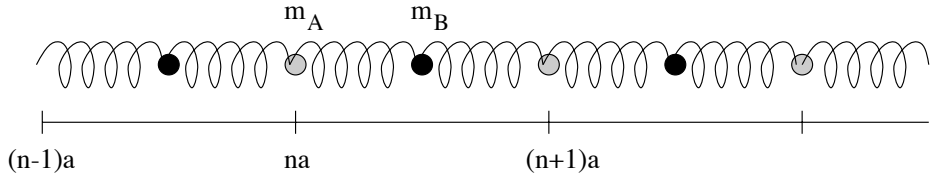


Figure 1.6: Lattice with two atoms of mass m_A and m_B per unit cell.

2. In lattices with two atoms (of different mass m_A and m_B) per unit cell (see Fig. 1.6) the spectrum of elementary phonon excitations splits into an **acoustic** and **optic** branch. For this model, show that the discrete lattice Lagrangian for a periodic system with $2 \times N$ masses can be written as

$$L = \sum_{n=1}^{N} \left[\frac{m_A}{2} (\dot{\phi}_n^{(A)})^2 + \frac{m_B}{2} (\dot{\phi}_n^{(B)})^2 - \frac{k_s}{2} \left(\phi_{n+1}^{(A)} - \phi_n^{(B)} \right)^2 - \frac{k_s}{2} \left(\phi_n^{(B)} - \phi_n^{(A)} \right)^2 \right].$$

Applying the Euler-Lagrange equation for the discrete model, obtain the classical equations of motion. Switching to the discrete Fourier representation (cf. Problem 1), $\phi_k^{(A/B)} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikna} \phi_n^{(A/B)}$ where $k = 2\pi m/a$ (m integer), show that the exact eigenspectrum, ω_k, can be obtained from the solution of the 2×2 secular equation for each k value

$$\det \begin{vmatrix} m_A \omega_k^2 - 2k_s & k_s(1 + e^{-ika}) \\ k_s(1 + e^{ika}) & m_B \omega_k^2 - 2k_s \end{vmatrix} = 0.$$

By finding an expression for the spectrum, obtain the asymptotic dependence as $k \to 0$. In this limit, describe qualitatively the symmetry of the normal modes.

---

3. Applying the Euler-Lagrange equation, obtain the equation of motion associated with the Lagrangian densities:

   1. $\mathcal{L}[\phi] = \frac{m\dot{\phi}^2}{2} - \frac{k_s a^2}{2} (\partial_x \phi)^2 - \frac{m}{2} \omega^2 \phi^2$
   2. $\mathcal{L}[\phi] = \frac{m\dot{\phi}^2}{2} - \frac{\kappa}{2} \left(\partial_x^2 \phi \right)^2$

3. $\mathcal{L}[\phi] = \frac{m\dot{\phi}^2}{2} - \frac{m}{2}\omega^2\phi^2 - \frac{\eta}{4}\phi^4$

4. $\mathcal{L}[\{\dot{\phi}_i\}] = \sum_{i=1}^{n}\left[\frac{m}{2}\dot{\phi}_i^2 - \frac{1}{2}k_s a^2(\partial_x\phi_i)^2\right]$

5. $\mathcal{L}[\dot{\phi}] = \frac{m}{2}|\dot{\phi}|^2 - \frac{1}{2}k_s a^2|\partial_x\phi|^2$

[Note that in 5. the field ϕ is complex.] Suggest a physical significance of the last term in 1. What is the effect of this term on the excitation spectrum of the corresponding quantum Hamiltonian? Starting with the Lagrangian 2., obtain the Hamiltonian density.

---

4. Following the discussion in the lectures, a periodic one-dimensional quantum elastic chain of length L is expressed by the Hamiltonian

$$\hat{H} = \int dx \left[\frac{1}{2m}\hat{\pi}^2 + \frac{k_s a^2}{2}(\partial_x\hat{\phi})^2\right]$$

where the field operators obey the canonical commutation relations

$$\left[\hat{\pi}(x), \hat{\phi}(x')\right] = -i\hbar\delta(x - x').$$

(a) Defining the Fourier representation,

$$\begin{Bmatrix}\hat{\phi}_k \\ \hat{\pi}_k\end{Bmatrix} \equiv \frac{1}{L^{1/2}}\int_0^L dx e^{\{\mp ikx}\begin{Bmatrix}\hat{\phi}(x) \\ \hat{\pi}(x)\end{Bmatrix}, \qquad \begin{Bmatrix}\hat{\phi}(x) \\ \hat{\pi}(x)\end{Bmatrix} = \frac{1}{L^{1/2}}\sum_k e^{\{\pm ikx}\begin{Bmatrix}\hat{\phi}_k \\ \hat{\pi}_k\end{Bmatrix},$$

where $\sum_k$ represents the sum over all quantised quasi-momenta $k = 2\pi m/L$, $m \in \mathcal{Z}$, show that the field operators obey the commutation relations $[\hat{\pi}_k, \hat{\phi}_{k'}] = -i\hbar\delta_{kk'}$.

(b) In the Fourier representation, show that the Hamiltonian takes the form

$$\hat{H} = \sum_k \left[\frac{1}{2m}\hat{\pi}_k\hat{\pi}_{-k} + \frac{k_s a^2}{2}k^2\hat{\phi}_k\hat{\phi}_{-k}\right].$$

(c) Defining

$$a_k \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_k + i\frac{1}{m\omega_k}\hat{\pi}_{-k}\right)$$

where $\omega_k = a(k_s/m)^{1/2}|k| = v|k|$ show that the field operators obey the canonical commutation relations $[a_k, a_{k'}^\dagger] = \delta_{kk'}$, and $[a_k, a_{k'}] = 0$.

(d) Finally, with this definition, show that the Hamiltonian can be expressed in the form

$$\hat{H} = \sum_k \hbar\omega_k\left(a_k^\dagger a_k + \frac{1}{2}\right).$$

1.3.2 Answers

1. Applying the Euler-Lagrange equation $d_t(\partial_{\dot{\phi}_n} L) - \partial_{\phi_n} L = 0$ to the discrete Lagrangian of the lattice model, one finds that the N equations of motion take the form of a three-term difference equation,[14]

$$m\ddot{\phi}_n = k_s \left(\phi_{n+1} - 2\phi_n + \phi_{n-1}\right).$$

As in the continuum theory, the latter can be brought to diagonal form by turning to the Fourier representation. Applying the *Ansatz*

$$\phi_n(t) = \frac{1}{\sqrt{N}} \sum_k e^{-i(\omega_k t - kna)} \phi_k$$

where the discrete quasi-momenta $k = 2\pi m/Na$ take values from the range $m = [-N/2, N/2]$ (i.e. the first **Brillouin zone**), we find $[m\omega_k^2 - 2k_s(1-\cos(ka))]\phi_k = 0$. From this equation one obtains the dispersion relation

$$\omega_k = 2\sqrt{\frac{k_s}{m}} |\sin(ka/2)|.$$

For $k \to 0$, this result collapses to the linear dispersion relation $\omega_k = v|k|$ obtained from the continuum theory. This can be understood simply by comparing the wavelength of the lattice vibration $\lambda = 2\pi/k$ with the lattice spacing a. When $\lambda \gg a$, the *relative* displacement of the atomic sites is small and the continuum approximation is justified. When $\lambda \sim a$, the relative displacement is large and the continuum theory becomes inapplicable.

---

2. Applying the Euler-Lagrange equations we obtain the $2 \times N$ coupled equations of motion

$$\begin{aligned} m_A \ddot{\phi}_n^{(A)} &= k_s \left(\phi_n^{(B)} - 2\phi_n^{(A)} + \phi_{n-1}^{(B)}\right), \\ m_B \ddot{\phi}_n^{(B)} &= k_s \left(\phi_{n+1}^{(A)} - 2\phi_n^{(B)} + \phi_n^{(A)}\right). \end{aligned}$$

[14] Note that, looking for stationary solutions $\phi_n(t) = e^{-i\omega t}$, the difference equation can be written as the eigenvalue equation $m\omega^2\phi_n = \sum_m^N M_{nm}\phi_n$, where

$$M = k_s \begin{pmatrix} \cdots & \cdots & \cdots & & & 0 \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ 0 & & & \cdots & \cdots & \cdots \end{pmatrix}.$$

The latter has eigenfunctions corresponding to the discrete Fourier transform: i.e. writing the eigenvalue equation as $m\omega^2|n\rangle = \hat{M}|n\rangle$, the normalised eigenfunctions $|k\rangle$, indexed by the wavenumber $k \in [-\pi/a, \pi/a]$, are given by $\phi_n(k) \equiv \langle n|k\rangle = \frac{1}{\sqrt{N}} e^{ikna}$. Later, in the next chapter, we will see that these eigenfunctions (of the discrete lattice Laplacian) will present a convenient basis for expansion of more complicated lattice models.

Applying the *Ansatz* $\phi_n^{(A/B)} = \frac{1}{\sqrt{N}} \sum_k e^{-i(\omega_k t - kna)} \phi_k^{(A/B)}$, one obtains

$$\begin{pmatrix} m_A\omega_k^2 - 2k_s & k_s(1+e^{-ika}) \\ k_s(1+e^{ika}) & m_B\omega_k^2 - 2k_s \end{pmatrix} \begin{pmatrix} \phi_k^{(A)} \\ \phi_k^{(B)} \end{pmatrix} = 0.$$

Diagonalizing the 2×2 matrix one recovers the secular equation shown in the question and from which we obtain the dispersion relation (see Fig. 1.9)

$$\omega_k^{(\pm)} = \omega_0 \left[1 \pm \left(1 - \frac{4m_A m_B}{(m_A+m_B)^2} \sin^2(ka/2) \right)^{1/2} \right]^{1/2},$$

where $\omega_0 = \sqrt{k_s/\mu}$ and $\mu = 1/(m_A^{-1} + m_B^{-1})$ denotes the reduced mass.

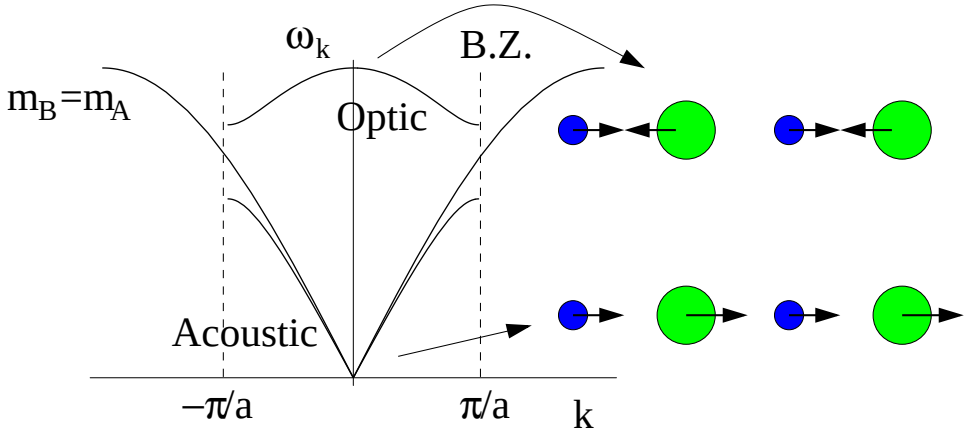


Figure 1.9: Spectrum of the two-atom discrete linear chain. Note that when $m_A = m_B$ we recover the spectrum of the single atom chain with period $a/2$. For $m_A \neq m_B$, a gap opens at the Brillounin zone boundary. The lower energy band is known as the acoustic branch where atoms in each unit cell move in phase. The higher energy optic branch involves atoms in each cell moving in antiphase.

An expansion in the limit $k \to 0$ yields

$$\omega_k^{(\pm)} \to \omega_0 \begin{cases} \sqrt{2}\left(1 - \dfrac{m_A m_B}{8(m_A+m_B)^2}(ka)^2\right) + O(k^4) \\ \sqrt{\dfrac{m_A m_B}{2}} \dfrac{1}{(m_A+m_B)} |ka| + O(k^3) \end{cases}$$

from which we deduce that the lower branch describes acoustic phonons with a linear dispersion relation, while the optic phonons are massive with a quadratic spectrum.

---

3. To complete this problem, one must generalise the Euler-Lagrange equation derived in lectures. E.g., for case 2., a variation of the action obtains

$$\begin{aligned} \delta S &= \int \left[\mathcal{L}(\dot\phi + \epsilon\dot\eta, \partial_x^2\phi + \epsilon\partial_x^2\eta) - \mathcal{L}(\dot\phi, \partial_x^2\phi) \right] \\ &= \epsilon \int \left[\dot\eta \partial_{\dot\phi}\mathcal{L} + \partial_x^2\eta \partial_{\partial_x^2\phi}\mathcal{L} \right] = \epsilon \int \eta \left[-d_t\partial_{\dot\phi}\mathcal{L} + d_x^2 \left(\partial_{\partial_x^2\phi}\mathcal{L} \right) \right] \end{aligned}$$

from which we obtain the Euler-Lagrange equation

$$-d_t\partial_{\dot\phi}\mathcal{L} + d_x^2\left(\partial_{\partial_x^2\phi}\mathcal{L}\right) = 0.$$

Applied to the Lagrangian functionals at hand, one finds the equation of motion

1. $\ddot\phi - \dfrac{k_s a^2}{m}\partial_x^2\phi + \omega^2\phi = 0,$
2. $\ddot\phi + \dfrac{\kappa}{m}\partial_x^4\phi = 0,$
3. $\ddot\phi + \omega^2\phi + \dfrac{\eta}{m}\phi^3 = 0$
4. $\ddot\phi_i - \dfrac{k_s a^2}{m}\partial_x^2\phi_i = 0.$

Finally, turning to case 5., it is necessary to generalise the Euler-Lagrange equation to account for complex fields. Since the real and imaginary parts fluctuate independently, we can consider a variation of each independently. Separating $\phi = \phi' + i\phi''$ into its real and imaginary parts, and applying a variation to each component, one obtains

$$\ddot\phi' - \frac{k_s a^2}{m}\partial_x^2\phi' = 0, \qquad \ddot\phi'' - \frac{k_s a^2}{m}\partial_x^2\phi'' = 0.$$

In fact, this result shows that the components ϕ and the complex conjugate ϕ^* can be treated as independent. A variation of the action with respect to ϕ^* obtains

5. $\ddot\phi - \dfrac{k_s a^2}{m}\partial_x^2\phi = 0.$

Physically, one can interpret the last term in 1. as a harmonic lattice binding potential. Its effect is to render the fluctuations massive, viz. $\omega_k = \sqrt{\omega^2 + v^2k^2}$.

For case 2. the momentum conjugate to the field ϕ is given by $\pi = \partial_{\dot\phi}\mathcal{L} = m\dot\phi$. The Hamiltonian corresponding to case 2. is given by

$$\mathcal{H} = \pi\dot\phi - \mathcal{L} = \frac{\pi^2}{2m} + \frac{k_s a^2}{2}(\partial_x^2\phi)^2.$$

---

4. (a) Using the definition provided, together with the canonical commutation relations of the field operators, one obtains

$$[\hat\pi_k, \hat\phi_{k'}] = \frac{1}{L}\int_0^L dx \int_0^L dx' e^{ikx - ik'x'} \overbrace{[\hat\pi(x), \hat\phi(x')]}^{-i\hbar\delta(x-x')} = -i\hbar \overbrace{\frac{1}{L}\int_0^L dx\ e^{i(k-k')x'}}^{\delta_{kk'}} = -i\hbar\delta_{kk'}.$$

(b) Again, using the definition, the kinetic component of the Hamiltonian takes the form

$$\int_0^L dx\ \frac{\hat\pi^2}{2m} = \sum_{kk'}\frac{1}{L}\int_0^L dx\ e^{-i(k+k')x}\frac{1}{2m}\ \hat\pi_k\hat\pi_{k'} = \sum_k \frac{1}{2m}\hat\pi_k\hat\pi_{-k}.$$

Similarly, applied to the potential component one obtains the Hamiltonian as advertised.

(c) Using the commutation relation derived above, one finds

$$[a_k, a^\dagger_{k'}] = \frac{i}{2\hbar}\left([\hat{\phi}_{-k}, \hat{\pi}_{-k'}] - [\hat{\pi}_k \hat{\phi}_{k'}]\right) = \delta_{kk'}, \qquad [a^\dagger_k, a^\dagger_{k'}] = 0.$$

(d) Inverting the expression for the field operators, one finds

$$\hat{\phi}_k = \left(\frac{\hbar}{2m\omega_k}\right)^{1/2}\left(a_k + a^\dagger_{-k}\right), \qquad \hat{\pi}_k = i\left(\frac{m\hbar\omega_k}{2}\right)^{1/2}\left(a^\dagger_k - a_{-k}\right).$$

Using the identity

$$\begin{aligned}\frac{1}{2m}\left(\hat{\pi}_k\hat{\pi}_{-k} + \hat{\pi}_{-k}\hat{\pi}_k\right) + \frac{k_s a^2}{2}k^2\left(\hat{\phi}_k\hat{\phi}_{-k} + \hat{\phi}_{-k}\hat{\phi}_k\right) \\ = \frac{1}{2}\hbar\omega_k\left(a^\dagger_k a_k + a_k a^\dagger_k + a^\dagger_{-k}a_{-k} + a_{-k}a^\dagger_{-k}\right).\end{aligned}$$

together with the commutation relations, after summation over k, we obtain the harmonic oscillator Hamiltonian.

2.4 Problem Set

2.4.1 Questions on the Second Quantisation

1. (a) Starting with the commutation relation for bosonic creation $a^\dagger$ and annihilation operators a, $\left[a, a^\dagger\right]_- = 1$, show that

$$[a^\dagger a, a]_- = -a, \qquad [a^\dagger a, a^\dagger]_- = a^\dagger.$$

Using this result, show that, if $|\alpha\rangle$ represents an eigenstate of the operator $a^\dagger a$ with eigenvalue α, $a|\alpha\rangle$ is also an eigenstate with eigenvalue $(\alpha-1)$ (unless $a|\alpha\rangle = 0$). Similarly, show that $a^\dagger|\alpha\rangle$ is an eigenstate with eigenvalue $(\alpha+1)$.

(b) If $|\alpha\rangle$ represents a normalised eigenstate of the operator $a^\dagger a$ with eigenvalue α for all $\alpha \geq 0$, show that

$$a|\alpha\rangle = \sqrt{\alpha}|\alpha-1\rangle\,, \qquad a^\dagger|\alpha\rangle = \sqrt{\alpha+1}|\alpha+1\rangle\,.$$

[Hint: consider the norm of the state.] Defining $|\Omega\rangle$ the normalised vacuum state, annihilated by the operator a, show that $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|\Omega\rangle$ is a normalised eigenstate of $a^\dagger a$ with eigenvalue n.

As an additonal exercise, consider the generalisation of parts (a) and (b) to the case of fermionic operators a.

---

2. Starting from first principles, show that the second quantised representation of the one-body kinetic energy operator is given by

$$\hat{T} = \int_0^L dx\; a^\dagger(x)\frac{\hat{p}^2}{2m}a(x).$$

[Hint: it may be helpful to start with the Fourier representation in which the one-body kinetic energy operator is diagonal and carefully transform to the real space basis.]

---

3. Transforming to the Fourier basis, show that the non-interacting three-dimensional cubic lattice tight-binding Hamiltonian,

$$\hat{H}^{(0)} = -t\sum_{\langle \mathbf{mn}\rangle}\left(c^\dagger_{\mathbf{m}\sigma}c_{\mathbf{n}\sigma} + \text{h.c.}\right),$$

assumes a diagonal form. Here $\langle \mathbf{mn}\rangle$ denotes the sum over all neighbouring sites and h.c. is short-hand for the Hermitian conjugate.

---

4. Show that the Holstein-Primakoff transformation,

$$\hat{S}^- = a^\dagger\left(2S - a^\dagger a\right)^{1/2}, \qquad \hat{S}^+ = (\hat{S}^-)^\dagger\,, \qquad \hat{S}^z = S - a^\dagger a\,,$$

is consistent with the quantum spin algebra $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$. [Hint: you may prove this result without explicitly expansion of the square root!]

---

5. Confirm that the bosonic commutation relations of the operators α and $\alpha^\dagger$ are preserved by the Bogoluibov transformation,

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta & -\sinh\theta \\ -\sinh\theta & \cosh\theta \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}.$$

How and why is this transformation related to the Lorentz transformation?

---

6. (a) Making use of the spin commutation relation, $[\hat{S}^\alpha_m, \hat{S}^\beta_n] = i\delta_{mn}\epsilon^{\alpha\beta\gamma}\hat{S}^\gamma_m$ ($\hbar = 1$), apply the identity $i\dot{\hat{\mathbf{S}}}_i = [\hat{\mathbf{S}}_i, \hat{H}]$, to express the equation of motion of a spin in a nearest neighbour spin S one-dimensional Heisenberg ferromagnet, $\hat{H} = -J\sum_m \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}$.

(b) Interpreting the spins as *classical* vectors, and taking the continuum limit, show that the equation of motion of the *hydrodynamic modes* takes the form

$$\dot{\mathbf{S}} = Ja^2\mathbf{S} \times \partial^2\mathbf{S},$$

where a denotes the lattice spacing. [Hint: in transferring to the continuum limit, apply a Taylor expansion to the spins viz. $S_{m+1} = S_m + a\partial S_m + \frac{a^2}{2}\partial^2 S_m + \cdots$.]

(c) Confirm that the equation of motion is solved by the *Ansatz*, $\mathbf{S}(x,t) = (c\cos(kx - \omega t), c\sin(kx - \omega t), \sqrt{S^2 - c^2})$, and determine the dispersion. Sketch a 'snapshot' configuration of the spins in the chain.

---

7. †**Valence Bond Solid**: Starting with the spin 1/2 Majumdar-Ghosh Hamiltonian

$$\hat{H}_{\rm MG} = \frac{4|J|}{3}\sum_{n=1}^{N}\left(\hat{\mathbf{S}}_n \cdot \hat{\mathbf{S}}_{n+1} + \frac{1}{2}\hat{\mathbf{S}}_n \cdot \hat{\mathbf{S}}_{n+2}\right) + \frac{N|J|}{2},$$

where the total number of sites N is even, and $\hat{\mathbf{S}}_{N+1} = \hat{\mathbf{S}}_1$, show that the two dimer or valence bond states $|\Omega_\pm\rangle = \otimes\prod_{n=1}^{N/2}\frac{1}{\sqrt{2}}(|\uparrow\rangle_{2n}\otimes|\downarrow\rangle_{2n\pm1} - |\downarrow\rangle_{2n}\otimes|\uparrow\rangle_{2n\pm1})$, are exact ground states, i.e. $|\Omega_+\rangle$ describes the state where neighbouring spins on sites $2n$ and $2n+1$ are in a total spin singlet ($S = 0$) state. [Hint: recast the Hamiltonian in terms of the total spin of a triad $\hat{\mathbf{J}}_n = \hat{\mathbf{S}}_{n-1} + \hat{\mathbf{S}}_n + \hat{\mathbf{S}}_{n+1}$, and consider what this representation implies.] Consider what would happen if the total number of sites was odd.

---

8. **Su-Shrieffer-Heeger Model:** Polyacetylene consists of bonded CH groups forming an isomeric long chain polymer. According to molecular orbital theory, the carbon atoms are expected to be sp^2 hybridised suggesting a planar configuration of the molecule. An unpaired electron is expected to occupy a single p-orbital which points out of the plane. The weak overlap of the p-orbitals delocalise the electrons into a π-conduction band (cf. benzene) — see Fig. 2.13a. Therefore, according to the nearly free electron theory, one might expect the half-filled conduction band of a polyacetylene chain to be metallic. However, the energy of a half-filled band of a one-dimension system can always be lowered by imposing a periodic lattice distortion known as the **Peirels instability** (see Fig. 2.13b).

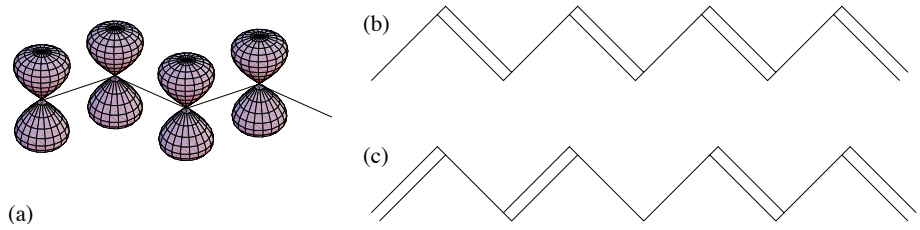


Figure 2.13: (a) Schematic diagram showing the π-bonding orbitals in long chain polyacetylene. (b) One of the configurations of the Peierls distorted chain. The double bonds represent the short links of the lattice. (c) A topological defect separating a two domains of the ordered phase.

One can think of an enhanced probability of finding the π electron on the short bond where the orbital overlap is stronger — the "double bond". The aim of this problem is to explore the instability.

(a) At its simplest level, the conduction band of polyacetylene can be modelled by a simple Hamiltonian, due to Su-Shrieffer-Heeger, in which the hopping matrix elements of the electrons are modulated by the lattice distortion of the atoms. Taking the displacement of the atomic sites from the equilibrium separation $a \equiv 1$ to be u_n, and treating their dynamics as classical, the effective Hamiltonian takes the form

$$\hat{H} \;=\; -t\sum_{n=1}^{N}\sum_{\sigma}(1+u_n)\left[c^{\dagger}_{n\sigma}c_{n+1\sigma}+\text{h.c.}\right]+\sum_{n=1}^{N}\frac{k_s}{2}\left(u_{n+1}-u_n\right)^2,$$

where, for simplicity, the boundary conditions are taken to be periodic. The first term describes the hopping of electrons between neighbouring sites with a matrix element modulated by the periodic distortion of the bond-length, while the last term represents the associated increase in the elastic energy. Taking the lattice distortion to be periodic, $u_n = (-1)^n\alpha$, and the *number of sites to be even*, diagonalise the Hamiltonian. [Hint: the lattice distortion lowers the symmetry of the lattice. The Hamiltonian is most easily diagonalised by distinguishing the two sites of the sublattice — i.e. doubling the size of the elementary unit cell — and transforming to the Fourier representation.] Show that the Peierls distortion of the lattice opens a gap in the spectrum at the Fermi level of the half-filled system.

(b) By estimating the total electronic and elastic energy of the half-filled band (i.e. an average of one electron per lattice site), show that the one-dimensional system is always unstable towards the Peierls distortion. To complete this calculation, you will need the approximate formula for the (elliptic) integral,

$$\int_{-\pi/2}^{\pi/2} dk\left(1-\left(1-\alpha^2\right)\sin^2 k\right)^{1/2} \simeq 2+(a_1-b_1\ln\alpha^2)\alpha^2$$

where a_1 and b_1 are (unspecified) numerical constants.

†(c) For an even number of sites, the Peierls instability has two degenerate configurations (see Fig. 2.13b) — ABABAB.. and BABABA... Comment on the qualitative form of the ground state lattice configuration if the number of sites is odd (cf. Fig. 2.13c).

---

9. In the **Schwinger boson representation** quantum mechanical spin is expressed in terms of two bosonic operators, a and b, in the form $\hat{S}^+ = a^\dagger b$, $\hat{S}^- = (\hat{S}^+)^\dagger$, $\hat{S}^z = \frac{1}{2}(a^\dagger a - b^\dagger b)$.

   (a) Show that this definition is consistent with spin commutation relations $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$.

   (b) Using the bosonic commutation relations, show that

$$|S, m\rangle = \frac{(a^\dagger)^{S+m}}{\sqrt{(S+m)!}} \frac{(b^\dagger)^{S-m}}{\sqrt{(S-m)!}} |\Omega\rangle,$$

   is compatible with the definition of an eigenstate of the total spin operator $\hat{\mathbf{S}}^2$ and $\hat{S}^z$. Here $|\Omega\rangle$ denotes the vacuum of the Schwinger bosons, and the total spin S defines the physical subspace $\{|n_a, n_b\rangle : n_a + n_b = 2S\}$.

---

10. †**The Jordan-Wigner Transformation**: So far we have shown how the algebra of quantum mechanical spin can be expressed using boson operators. Here we show that a representation for spin 1/2 can be obtained in terms of Fermion operators. Specifically, let us represent an up spin as a particle and a down spin as the vacuum $|0\rangle$, viz. $|\uparrow\rangle \equiv |1\rangle = f^\dagger|0\rangle$, and $|\downarrow\rangle \equiv |0\rangle = f|1\rangle$. In this representation the spin raising and lowering operators are expressed in the form $\hat{S}^+ = f^\dagger$ and $\hat{S}^- = f$, while $\hat{S}^z = f^\dagger f - 1/2$.

    (a) With this definition, confirm that the spins obey the algebra $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$.

    However, there is a problem: spins on different sites commute while fermion operators anticommute, e.g. $S_i^+ S_j^+ = S_j^+ S_i^+$, but $f_i^\dagger f_j^\dagger = -f_j^\dagger f_i^\dagger$. To obtain a faithful spin representation, it is necessary cancel this unwanted sign. Although a general procedure is hard to formulate, in one dimension, this can be achieved by a non-linear transformation, viz.

$$\hat{S}_l^+ = f_l^\dagger e^{i\pi \sum_{j<l} \hat{n}_j}, \qquad \hat{S}_l^- = e^{-i\pi \sum_{j<l} \hat{n}_j} f_l, \qquad \hat{S}_l^z = f_l^\dagger f_l - \frac{1}{2}.$$

    Operationally, this seemingly complicated transformation has a straightforward interpretation: in one dimension, the particles can be ordered on the line. By counting the number of particles 'to the left' we can assign an overall phase of $+1$ or -1 to a given configuration and thereby transmute the particles into a fermions. (Put differently, the exchange to two fermions induces a sign change which is compensated by the factor arising from the phase — the 'Jordan-Wigner string'.)

    (b) Using the Jordan-Wigner representation, show that $\hat{S}_m^+ \hat{S}_{m+1}^- = f_m^\dagger f_{m+1}$.

    (c) For the spin 1/2 anisotropic quantum Heisenberg spin chain, the spin Hamiltonian assumes the form

$$\hat{H} = -\sum_n \left[J_z \hat{S}_n^z \hat{S}_{n+1}^z + \frac{J_\perp}{2} \left(\hat{S}_n^+ \hat{S}_{n+1}^- + \hat{S}_n^- \hat{S}_{n+1}^+ \right) \right].$$

    Turning to the Jordan-Wigner representation, show that the Hamiltonian can be cast in the form

$$\hat{H} = -\sum_n \left[\frac{J_\perp}{2} \left(f_n^\dagger f_{n+1} + \text{h.c.} \right) + J_z \left(\frac{1}{4} - f_n^\dagger f_n + f_n^\dagger f_n f_{n+1}^\dagger f_{n+1} \right) \right].$$

    (d) The mapping above shows that the one-dimensional quantum spin 1/2 XY-model (i.e. $J_z = 0$) can be diagonalised as a non-interacting theory of spinless fermions. In this case, show that the spectrum assumes the form $\epsilon_k = -J_\perp \cos ka$.

2.4.2 Answers

1. (a) Making use of the commutation relations for bosons, one finds

$$a^\dagger aa = a(a^\dagger a - 1), \qquad a^\dagger aa^\dagger = a^\dagger(1 + a^\dagger a)$$

from which the results follow. Using these results, one finds that, providing $a|\alpha\rangle \neq 0$,

$$\begin{aligned} a^\dagger a\ a|\alpha\rangle &= a(a^\dagger a - 1)|\alpha\rangle = (\alpha - 1)a|\alpha\rangle \\ a^\dagger a\ a^\dagger|\alpha\rangle &= a^\dagger(1 + a^\dagger a)|\alpha\rangle = (1 + \alpha)a^\dagger|\alpha\rangle \end{aligned}$$

(b) If $|\alpha\rangle$ is a normalised eigenstate of $a^\dagger a$ with eigenvalue α, the norm of state created by the action of the creation operator is given by

$$||a^\dagger|\alpha\rangle|| \equiv \sqrt{\langle\alpha|aa^\dagger|\alpha\rangle} = \sqrt{\langle\alpha|a^\dagger a + 1|\alpha\rangle} = \sqrt{\alpha + 1}.$$

Similarly, the norm of state created by the action of the annihilation operator is given by

$$||a|\alpha\rangle|| \equiv \sqrt{\langle\alpha|a^\dagger a|\alpha\rangle} = \sqrt{\alpha}.$$

Therefore, if we define $|\alpha + 1\rangle$ and $|\alpha - 1\rangle$ as the normalised eigenstates of the operator $a^\dagger a$ with eigenvalue $\alpha + 1$ and $\alpha - 1$ respectively, one finds

$$\begin{aligned} a|\alpha\rangle &= \sqrt{\alpha}|\alpha - 1\rangle \\ a^\dagger|\alpha\rangle &= \sqrt{\alpha + 1}|\alpha + 1\rangle \end{aligned}$$

Defining as the vacuum $|\Omega\rangle$ the normalised state that is annihilated by the operator a, an application of the result above shows the state $|n\rangle = (1/\sqrt{n!})(a^\dagger)^n|\Omega\rangle$ to be a normalised eigenstate of $a^\dagger a$ with eigenvalue n.

---

2. The kinetic energy operator is diagonal in the momentum basis. Following the analysis in the text, the corresponding second quantised one-body operator is given by $\hat{T} = \sum_p \frac{p^2}{2m} a_p^\dagger a_p$. Transforming to the coordinate representation, $a_p = L^{-1/2} \int_0^L dx e^{ipx/\hbar} a(x)$, one obtains

$$\hat{T} = \frac{1}{L} \sum_p \frac{p^2}{2m} \int_0^L dy \int_0^L dx e^{ip(x-y)/\hbar} a^\dagger(y) a(x).$$

Expressing factor p^2 as a derivative of the exponential factor, and integrating by parts, one obtains the required result.

---

3. A Hamiltonian which is translationally invariant is easily diagonalised in the Fourier representation. Setting $c^\dagger_{\mathbf{m}\sigma} = \frac{1}{N^{d/2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{m}} c^\dagger_{\mathbf{k}\sigma}$, the Hamiltonian takes the form

$$\hat{H}^{(0)} = \sum_{\mathbf{k}}^{\text{B.Z.}} \sum_{\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma},$$

where $\epsilon_{\mathbf{k}} = -t \sum_{i=x,y,z} e^{i\mathbf{k}\cdot\hat{\mathbf{e}}_i} = -2t \sum_{i=x,y,z} \cos(\mathbf{k}\cdot\hat{\mathbf{e}}_i)$, with the sum running over neighbouring lattice vectors $\hat{\mathbf{e}}_i$, and the lattice spacing is taken to be unity.

---

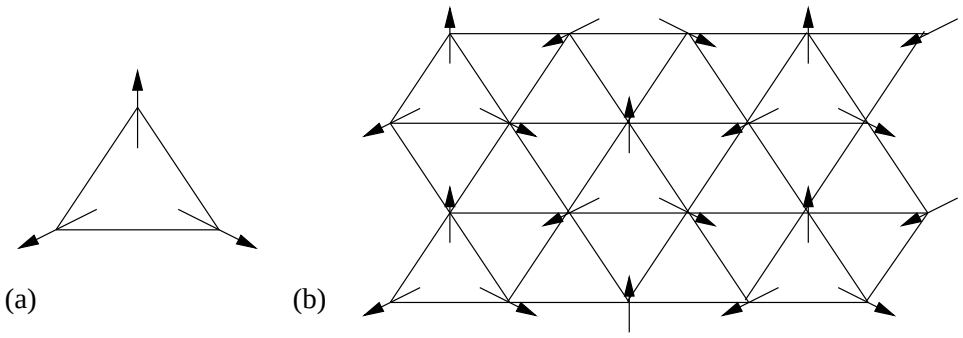
4. Substituting the definition of the spin raising and lowering operators using the Holstein-Primakoff transformation, the commutator is obtained as

$$\begin{aligned}\frac{1}{2S}[\hat{S}^+, \hat{S}^-] &= \left(1 - \frac{a^\dagger a}{2S}\right)^{1/2} \overbrace{a a^\dagger}^{1 + a^\dagger a} \left(1 - \frac{a^\dagger a}{2S}\right)^{1/2} - a^\dagger \left(1 - \frac{a^\dagger a}{2S}\right) a \\ &= \left(1 - \frac{a^\dagger a}{2S}\right) + a^\dagger a \left(1 - \frac{a^\dagger a}{2S}\right) - a^\dagger a + \frac{a^\dagger a^\dagger a a}{2S} = 1 - \frac{a^\dagger a}{S}.\end{aligned}$$

With $S^z = S - a^\dagger a$, we obtain the required commutation relation $[\hat{S}^+, \hat{S}^-] = 2S^z$.

---

5. By symmetry, the maximal exchange energy that can be recovered is obtained when the spins are maximally anti-aligned, i.e. at 120^o to each other. Using the spin



orientation of a single triangle, the two-dimensional triangular lattice can be tessilated with all spins aligned at 120^o to the neighbours. Notice that this configuration represents just one of an infinite degenerate manifold of ground states obtained by global rotation of the spins.

---

6. To confirm the validity of the Bogoluibov transformation let us consider the commutation relations of α:[27]

$$\begin{aligned}\left[\alpha, \alpha^\dagger\right] &= \left[\cosh\theta\ a + \sinh\theta\ a^\dagger, \cosh\theta\ a^\dagger + \sinh\theta\ a\right] \\ &= \cosh^2\theta\left[a, a^\dagger\right] + \sinh^2\theta\left[a^\dagger, a\right] = \cosh^2\theta - \sinh^2\theta = 1.\end{aligned}$$

as required.

---

7. (a) Making use of the equation of motion $i\dot{\hat{\mathbf{S}}}_i = [\hat{\mathbf{S}}_i, \hat{H}]$, and the commutation relation $[S_i^\alpha, S_j^\beta] = i\delta_{ij}\epsilon^{\alpha\beta\gamma}S_i^\gamma$, we obtain

$$i\dot{\hat{\mathbf{S}}}_i = Ji\hat{\mathbf{S}}_i \times \left(\hat{\mathbf{S}}_{i+1} + \hat{\mathbf{S}}_{i-1}\right)$$

(b) Interpreting the spins as classical vectors, and applying the Taylor expansion $\mathbf{S}_{i+1} = \mathbf{S}_i + a\partial\mathbf{S}_i + (a^2/2)\partial^2\mathbf{S}_i + \cdots$, we obtain the classical equation of motion

$$\dot{\mathbf{S}} = Ja^2\mathbf{S} \times \partial^2\mathbf{S}.$$

Substituting, we find that $\mathbf{S} = \left(c\cos(kx - \omega t), c\sin(kx - \omega t), \sqrt{S^2 - c^2}\right)$, satisfies the equation of motion with $\omega = J(ka)^2\sqrt{S^2 - c^2}$.

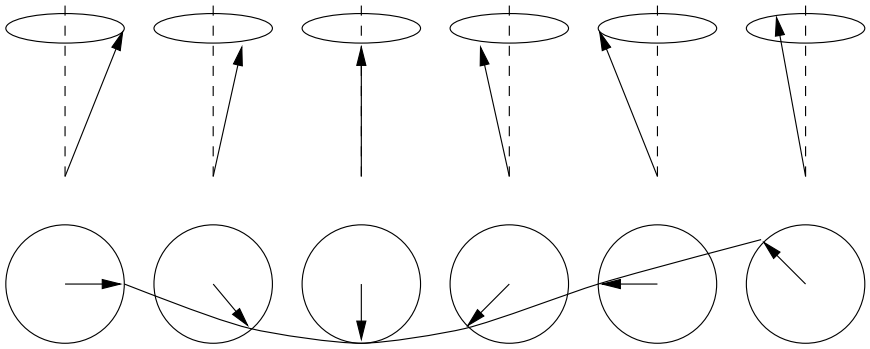


Figure 2.14: Spin-wave dispersion.

(c) The corresponding spin wave solution has the precessional form shown in Fig. 2.14.

---

[27] More formally, one may prove the relation as follows: Suppose we define a two component operator $\mathbf{a} = (a, a^\dagger)$. If a obeys bosonic commutation relations, $[a_\mu, a_\nu^\dagger] = g_{\mu\nu}$ where the diagonal matrix has elements $g = \mathrm{diag}(1, -1)$. If we define an operator transformation Λ such that $\alpha_\mu = \Lambda_{\mu\nu}a_\nu$ (summation convention implied), then the condition that the commutation relations are preserved requires

$$g_{\mu\nu} \stackrel{!}{=} [\alpha_\mu, \alpha_\nu^\dagger] = \Lambda_{\mu\eta}\Lambda^*_{\nu\gamma}[a_\eta, a_\gamma^\dagger] = \Lambda_{\mu\eta}\Lambda^*_{\nu\gamma}g_{\eta\gamma},$$

i.e. the admissable transformations fulfil the condition that $g_{\mu\nu} = \Lambda_{\mu\eta}\Lambda^*_{\nu\gamma}g_{\eta\gamma}$. Such transformations, that preserve the "metric" $g = \mathrm{diag}(1, -1)$, belong to the group of Lorentz transformations. In the context of bosonic operators, they are termed Bogoluibov transformations. Note that, for fermionic systems, with $\mathbf{c} = (c, c^\dagger)$, $[c_\mu, c_\nu^\dagger] = \delta_{\mu\nu}$. In this case, we require that $\delta_{\mu\nu} = \Lambda_{\mu\eta}\Lambda^*_{\nu\gamma}\delta_{\eta\gamma}$, i.e. Λ belongs the class of Unitary transformations: $\Lambda^\dagger\Lambda = \mathbf{1}$

8. Defining the total spin on a triad $\hat{\mathbf{J}}_n = \hat{\mathbf{S}}_{n-1} + \hat{\mathbf{S}}_n + \hat{\mathbf{S}}_{n+1}$, the Hamiltonian can be recast in the form

$$\hat{H}_{\rm MG} = |J| \sum_{n=1}^{N} \hat{\mathcal{P}}_{3/2}(n-1, n, n+1),$$

where $\hat{\mathcal{P}}_{3/2}(n-1,n,n+1) = (\hat{\mathbf{J}}_n^2 - 3/4)/3$ annihilates any state with total spin $J = 1/2$ of the triad. Since in any three sites, two of the spins are in a singlet, there can be no components of $J = 3/2$ on any triad. Therefore the dimer states are eigenstates of zero energy. Now since $\hat{\mathcal{P}}_{3/2}$ is positive definite, these states must be the ground states.

---

9. (a) Since each unit cell is of twice the dimension of the original lattice, we begin by recasting the Hamiltonian in the sublattice form

$$\hat{H} = -t \sum_{m=1,\sigma}^{N/2} \left\{ (1+\alpha) \left[a^\dagger_{m\sigma} b_{m\sigma} + \text{h.c.} \right] + (1-\alpha) \left[b^\dagger_{m\sigma} a_{m+1\sigma} + \text{h.c.} \right] \right\} + \frac{N k_s \alpha^2}{2}.$$

Switching to the Fourier basis, $a_m = \sqrt{2/N} \sum_k e^{-2ikm} a_k$ (similarly b_m), where k takes $N/2$ values uniformly on the interval $[-\pi/2, \pi/2]$, the Hamiltonian takes the form

$$\hat{H} = \frac{N k_s a^2}{2} \alpha^2 \\ -t \sum_{k\sigma} \begin{pmatrix} a^\dagger_{k\sigma} & b^\dagger_{k\sigma} \end{pmatrix} \begin{pmatrix} 0 & (1+\alpha) + (1-\alpha) e^{-2ik} \\ (1+\alpha) + (1-\alpha) e^{2ik} & 0 \end{pmatrix} \begin{pmatrix} a_{k\sigma} \\ b_{k\sigma} \end{pmatrix}.$$

Diagonalising the 2×2 Hamiltonian, we obtain the spectrum

$$\epsilon(k) = \pm 2t \left[\cos^2 k + \alpha^2 \sin^2 k \right]^{1/2}.$$

Reassuringly, in the limit $\alpha \to 0$, we obtain the cosine spectrum of the undistorted problem, while in the limit $\alpha \to 1$, pairs of monomers become decoupled and we obtain a massively degenerate bonding and antibonding spectrum.

(b) According to the formula given in the text, the total shift in energy is given by

$$\delta\epsilon = -2t(a_1 - b_1 \ln \alpha^2)\alpha^2 + \frac{N k_s \alpha^2}{2}$$

Maximising the energy gain with respect to α, one finds that the stable configuration is found when

$$\alpha^2 = \exp\left[\frac{a_1}{b_1} - 1 - \frac{N k_s}{4 t b_1} \right]$$

(c) If the number of sites is odd, the Peirels distortion is inevitably frustrated — a configuration that starts ABABAB must finish as BABABA. The result is that the polymer chain must accommodate a **topological excitation**. The excitation is said to be topological because the defect can not be removed by a smooth continuous deformation — it is like a dislocation line in a crystal. Its effect on the spectrum of the model is to introduce a state that lies within the band gap of the material.

The consideration of an odd number of sites forces a topological defect into the system. However, even if the number of sites is even, one can create low energy topological excitations of the system either by doping (see fig. 2.13c), or by the creation of **excitons**, particle-hole excitations of the system. Indeed, such topological excitations can dominate the transport properties of the system.

As a footnote, one should add that the particular model considered above is somewhat over-simplified. It seems likely that Coulomb interactions play a dominant role in driving the Peirels instability in Polyacetylene. However, the qualitative interpretation of the existence of topological excitations is born out by experiment.

---

10. (a) Using the commutation relation for bosons, one finds.

$$\begin{aligned}[\hat{S}^+, \hat{S}^-] &= a^\dagger b\; b^\dagger a - b^\dagger a\; a^\dagger b = a^\dagger a b b^\dagger - a a^\dagger b^\dagger b \\ &= a^\dagger a(b^\dagger b + 1) - (a^\dagger a + 1) b^\dagger b = a^\dagger a - b^\dagger b = 2\hat{S}^z.\end{aligned}$$

(b) Using the identity

$$\begin{aligned}\hat{\mathbf{S}}^2 &= (\hat{S}^z)^2 + \frac{1}{2}\left(\hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+\right) = \frac{1}{4}\left(\hat{n}_a - \hat{n}_b\right)^2 + \frac{1}{2}\left(a^\dagger b\; b^\dagger a + b^\dagger a\; a^\dagger b\right) \\ &= \frac{1}{4}\left(\hat{n}_a - \hat{n}_b\right)^2 + \hat{n}_a\hat{n}_b + \frac{1}{2}\left(\hat{n}_a + \hat{n}_b\right),\end{aligned}$$

one finds that

$$\hat{\mathbf{S}}^2|S,m\rangle = \left[m^2 + (S+m)(S-m) + S\right]|S,m\rangle = S(S+1)|S,m\rangle$$

as required. Similarly, one finds

$$\begin{aligned}\hat{S}^z|S,m\rangle &= \frac{1}{2}(n_a - n_b)|n_a = S+m, n_b = S-m\rangle \\ &= \frac{1}{2}\left[(S+m) - (S-m)\right]|S,m\rangle = m|S,m\rangle,\end{aligned}$$

showing $|S,m\rangle$ to be an eigenstate of the operator $\hat{S}^z$ with eigenvalue m.

As with the Holstein-Primakoff representation, the Schwinger boson represents yet another representation of quantum mechanical spin. Which representation is most convenient for the analysis of quantum spin models depends sensitively on the nature of the microscopic Hamiltonian.

---

11. (a) Using the fermionic anticommutation relations, one finds

$$\begin{aligned}[\hat{S}^+, \hat{S}^-]_- &= [f^\dagger, f]_- = f^\dagger f - f f^\dagger \\ &= 2f^\dagger f - 1 = 2\hat{S}^z.\end{aligned}$$

(b) Using the fact that the number operators on different sites commute, one finds

$$\hat{S}^+_m \hat{S}^-_{m+1} = f^\dagger_m e^{i\pi \sum_{j<m} n_j} e^{-i\pi \sum_{l<m+1} n_l} f_{m+1} = f^\dagger_m e^{-i\pi n_m} f_{m+1} = f^\dagger_m f_{m+1}$$

where here we have made use of the fact that, for fermionic particles $f^\dagger_m e^{-i\pi n_m} \equiv f^\dagger_m$.

(c) The fermion representation is simply obtained by substitution.

(d) With $J_z = 0$, the spin Hamiltonian assumes the form of a non-interacting tight-binding Hamiltonian

$$\hat{H} = -\frac{J_\perp}{2} \sum_n \left(f^\dagger_n f_{n+1} + \text{h.c.} \right).$$

This Hamiltonian, which has been encountered previously, is diagonalised in the Fourier space after which one obtains the cosine band dispersion.

3.5 Questions on the Path Integral

1. **Quantum Harmonic Oscillator:** As emphasized in lectures, the quantum harmonic oscillator provides a valuable arena in which to explore the Feynman path integral and methods of functional integration. Along with a small number of other precious examples, the path integral may be computed exactly, and the Feynman propagator explored rigorously.

   (a) Starting with the Feynman path integral, show that the propagator for the one–dimensional quantum Harmonic oscillator, $\hat{H} = \hat{p}^2/2m + m\omega^2\hat{q}^2/2$, takes the form

   $$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \left(\frac{m\omega}{2\pi i\hbar\sin\omega t}\right)^{1/2}\exp\left[\frac{i}{2\hbar}m\omega\left(\left[q_I^2+q_F^2\right]\cot\omega t - \frac{2q_Iq_F}{\sin\omega t}\right)\right] .$$

   Suggest why the propagator varies periodically on the time interval t, and explain the origin of the singularities at $t = n\pi/\omega$, $n = 1, 2, \ldots$. Taking the frequency $\omega \to 0$, show that the propagator for the free particle is recovered.

   (b) Show that, the wavepacket $\psi(q, t = 0) = (2\pi a)^{-1/4}\exp[-q^2/4a]$ remains Gaussian at all subsequent times. Obtain the width $a(t)$ as a function of time.

   (c) Semiclassical limit: Taking the initial wavepacket to be of the form

   $$\psi(q, t = 0) = (2\pi a)^{-1/4}\exp\left[\frac{i}{\hbar}mvq - \frac{1}{4a}q^2\right] ,$$

   (which corresponds to a wavepacket centered at an initial position $q = 0$ with a velocity v) find the wavepacket at times $t > 0$, and determine the mean position, mean velocity, and mean width as a function of time.

2. **Density Matrix:** Focusing on the quantum harmonic oscillator, here we explore how real–time dynamical information can be converted into quantum statistical information.

   Using the results of the previous question, obtain the density matrix $\rho(q, q') = \langle q|e^{-\beta\hat{H}}|q'\rangle$ for the harmonic oscillator at finite temperature, $\beta = 1/T$ ($k_{\rm B} = 1$). Obtain and comment on the asymptotics: (i) $T \ll \hbar\omega$ and (ii) $T \gg \hbar\omega$. [Hint: In the high temperature case, be sure to carry out the expansion in $\hbar\omega/T$ to second order.]

3. **Winding Numbers:** In lectures, we considered the application of the Feynman path integral to model systems where trajectories could be parameterised in terms of their harmonic (Fourier) expansion. However, very often, one is interested in applications of the path integral to spaces that are not simply connected. In this case, one must include classes of trajectories which can not be simply continued. Rather, trajectories are classified by their 'winding number' on the space. To illustrate the point, let us consider the application of the path integral to a particle on a ring.

(a) Starting with the Hamiltonian $\hat{H} = -\frac{1}{2I}\frac{\partial^2}{\partial\theta^2}$, where θ denotes an angle variable, show from first principles that the quantum partition function $\mathcal{Z} = \mathrm{tr}\, e^{-\beta\hat{H}}$ is given by

$$\mathcal{Z} = \sum_{n=-\infty}^{\infty} \exp\left[-\beta\frac{n^2}{2I}\right]. \tag{3.61}$$

(b) Formulated as a Feynman path integral, show that the quantum partition function can be cast in the form

$$\mathcal{Z} = \int_0^{2\pi} d\theta \sum_{m=-\infty}^{\infty} \int_{\substack{\theta(0)=\theta \\ \theta(\beta)=\theta(0)+2\pi m}} D\theta(\tau) \exp\left[-\frac{I}{2}\int_0^\beta d\tau\dot{\theta}^2\right].$$

(c) Varying the Eulidean action with respect to θ, show that the path integral is minimised by the classical trajectories $\bar{\theta}(\tau) = \theta + 2\pi m\tau/\beta$. Parametrising a general path as $\theta(\tau) = \bar{\theta}(\tau) + \eta(\tau)$, where $\eta(\tau)$ is a path with no net winding, show that

$$\mathcal{Z} = \mathcal{Z}_0 \sum_{m=-\infty}^{\infty} \exp\left[-\frac{I}{2}\frac{(2\pi m)^2}{\beta}\right], \tag{3.62}$$

where $\mathcal{Z}_0$ represents the quantum partition function for a free particle with open boundary conditions. Making use of the free particle propagator, show that $\mathcal{Z}_0 = \sqrt{I/2\pi\beta}$.

(d) Finally, making use of Poisson's summation formula, $\sum_m h(m) = \sum_n \int_{-\infty}^{\infty} d\phi\, h(\phi) e^{2\pi i n\phi}$, show that Eq. (3.62) coincides with Eq. (3.61).

4. †**Particle in a Periodic Potential:** In section 3.3.2 it was shown that the quantum probability amplitude for quantum mechanical tunneling can be expressed as a sum over instanton field configurations of the Euclidean action. By generalising this approach, the aim of the present problem is to explore quantum mechanical tunneling in a periodic potential. Such an analysis allows us to draw a connection to the problem of the Bloch spectrum.

(a) A quantum mechanical particle moves in a periodic lattice potential V with periodicity a. Taking the Euclidean action for the instanton connecting two neighbouring minima to be $S_{\mathrm{inst.}}$, express the Euclidean time propagator $G(ma, na; \tau)$, with m and n integer, as a sum over instanton and anti–instanton field configurations.

(b) Making use of the identity $\delta_{qq'} = \int_0^{2\pi} e^{i(q-q')\theta} d\theta/(2\pi)$ show that

$$G(ma, na; \tau) \sim e^{\omega\tau/2} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i(n-m)\theta} \exp\left[\frac{\Delta\epsilon\tau}{\hbar} 2\cos\theta\right],$$

where our notation is taken from section 3.3.2.

(c) Keeping in mind that, in the periodic system, the eigenfunctions are Bloch states $\psi_{p\alpha}(q) = e^{ipq}u_{p\alpha}(q)$ where $u_{p\alpha}(q + ma) \equiv u_{p\alpha}(q)$ denotes the periodic part of the Bloch function, show that the propagator is compatible with a spectrum of the lowest band $\alpha = 0$, $\epsilon_p = \hbar\omega/2 - 2\Delta\epsilon\cos(pa)$.

3.6 Answers

1. (a) Making use of the Feynman path integral, the propagator can be expressed as the functional integral,

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{q(0)=q_I}^{q(t)=q_F} Dq\, e^{iS[q]/\hbar}, \qquad S[q] = \int_0^t dt\, \frac{m}{2}\left(\dot{q}^2 - \omega^2 q^2\right) .$$

The evaluation of the functional integral over field configurations $q(t')$ is facilitated by parameterising the path in terms of fluctuations around the classical trajectory. Setting $q(t') = q_{\rm cl}(t') + r(t')$ where $q_{\rm cl}(t')$ satisfies the classical equation of motion $m\ddot{q}_{\rm cl} = -m\omega^2 q_{\rm cl}$, and applying the boundary conditions, one obtains the solution $q_{\rm cl}(t') = A\sin(\omega t') + B\cos(\omega t')$, with the coefficients $B = q_I$ and $A = q_F/\sin(\omega t) - q_I\cot(\omega t)$. Being Gaussian in q, the action separates as $S[q] = S[q_{\rm cl}] + S[r]$, where

$$\begin{aligned} S[q_{\rm cl}] &= \frac{m\omega^2}{2}\left[(A^2 - B^2)\frac{\sin(2\omega t)}{2\omega} + 2AB\frac{\cos(2\omega t) - 1}{2\omega}\right] \\ &= \frac{m\omega}{2}\left[(q_I^2 + q_F^2)\cot(\omega t) - \frac{2q_I q_F}{\sin(\omega t)}\right] . \end{aligned}$$

Finally, integrating over the fluctuations and applying the identity $z/\sin z = \prod_{n=1}^{\infty}(1 - z^2/\pi^2 n^2)^{-1}$ one obtains the required result, periodic in t with frequency ω, and singular at $t = n\pi/\omega$. In particular, a careful regularisation of the expression for the path integral shows that

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle \mapsto \begin{cases} \delta(q_F - q_I) & t = 2\pi n/\omega, \\ \delta(q_F + q_I) & t = \pi(2n+1)/\omega. \end{cases}$$

Physically, the origin of the singularity is clear: The harmonic oscillator is peculiar in having a spectrum with energies uniformly spaced in units of $\hbar\omega$. Noting the eigenfunction expansion $\langle q_F|e^{-i\hat{H}t\hbar}|q_I\rangle = \sum_n \langle q_F|n\rangle\langle n|q_I\rangle e^{-i\omega n t}$, this means that when $\hbar\omega \times t/\hbar = 2\pi \times$ integer there is a coherent superposition of the states and the initial state is recovered. Furthermore, since the ground state and its even integer descendents are symmetric while the odd states are antisymmetric, it is straightforward to prove the identity for the odd periods (exercise).

(b) Given the initial condition $\psi(q, t = 0)$, the time evolution of the wavepacket can be determined from the propagator as $\psi(q,t) = \int_{-\infty}^{\infty} dq' \langle q|e^{-i\hat{H}t/\hbar}|q'\rangle\psi(q', 0)$ from which one obtains

$$\psi(q,t) = J(t)\int_{-\infty}^{\infty} dq' \frac{1}{(2\pi a)^{1/4}} e^{-q'^2/4a} e^{\frac{i}{\hbar}\frac{m\omega}{2}\left([q^2+q'^2]\cot(\omega t) - \frac{2qq'}{\sin(\omega t)}\right)}$$

where $J(t)$ represents the time–dependent contribution arising from the fluctuations around the classical trajectory. Being Gaussian in q', the integral can be performed explicitly. Setting $\alpha = 1/2a - im\omega\cot(\omega t)/\hbar$, $\beta = im\omega q/(\hbar\sin(\omega t))$, and performing the Gaussian integral over q', one obtains

$$\psi(q,t) = J(t)\frac{1}{(2\pi a)^{1/4}}\sqrt{\frac{2\pi}{\alpha}} e^{\beta^2/2\alpha} \exp\left[\frac{i}{2\hbar} m\omega q^2 \cot(\omega t)\right]$$

where $\beta^2/2\alpha = -(1 + i\kappa\cot(\omega t))q^2/4a(t)$. Rearranging terms, it is straightforward to show that $\psi(q,t) = (2\pi a(t))^{-1/4}\exp[-\frac{q^2}{4a(t)}]e^{i\varphi(q,t)}$, where $a(t) = a[\cos^2(\omega t) + \kappa^{-2}\sin^2(\omega t)]$, $\kappa = 2am\omega/\hbar$ and $\varphi(q,t)$ represents a pure phase.[42] As required, under the action of the propagator, the normalisation of the wavepacket is preserved. (A graphical representation of the time evolution is shown in Fig. 3.13a.) Note that, if $a = \hbar/2m\omega$ (i.e. $\kappa = 1$), $a(t) = a$ for all times — i.e. it is a pure eigenstate.

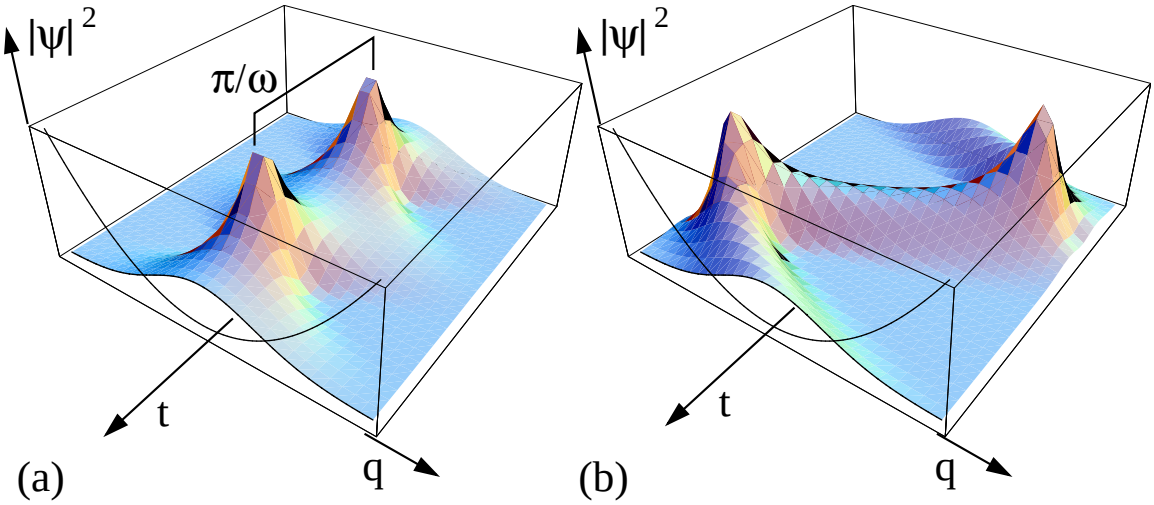


Figure 3.13: (a) Variation of a "stationary" Gaussian wavepacket in the harmonic oscillator taken from the solution, and (b) variation of the moving wavepacket.

(c) Still of a Gaussian form, the integration can again be performed explicitly for the new initial condition. In this case, we obtain an expression of the form above but with $\beta = \frac{i}{\hbar}\frac{m\omega}{\sin(\omega t)}(q - \frac{v}{\omega}\sin(\omega t))$. Reading off the coefficients, we find that the position and velocity of the wavepacket have the form $q_0(t) = (v/\omega)\sin(\omega t)$, $v(t) = v\cos(\omega t)$ coinciding with that of the classical dynamics. Note that, as above, the width $a(t)$ of the wavepacket oscillates at frequency ω. (A graphical representation of the time evolution is shown in Fig. 3.13b.)

2. The density matrix can be deduced from the general solution of the previous question. Turning to the Euclidean time formulation,

$$\begin{aligned}\rho(q,q') &= \langle q|e^{-\beta H}|q'\rangle = \langle q|e^{-(i/\hbar)H(\hbar\beta/i)}|q'\rangle \\ &= \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{1/2}\exp\left[-\frac{m\omega}{2\hbar}\left((q^2+q'^2)\coth(\beta\hbar\omega) - \frac{2qq'}{\sinh(\beta\hbar\omega)}\right)\right].\end{aligned}$$

(i) In the low temperature limit $T \ll \hbar\omega$ ($\beta\hbar\omega \gg 1$), $\coth(\beta\hbar\omega) \to 1$, $\sinh(\beta\hbar\omega) \to e^{\beta\hbar\omega}/2$, and

$$\rho(q,q') \simeq \left(\frac{m\omega}{\pi\hbar e^{\beta\hbar\omega}}\right)^{1/2}\exp\left[-\frac{m\omega}{2\hbar}(q^2+q'^2)\right] = \langle q|n=0\rangle\, e^{-\beta E_0}\,\langle n=0|q'\rangle\,.$$

[42] For completeness, we note that $\varphi(q,t) = -\frac{1}{2}\tan^{-1}(\frac{1}{\kappa}\cot(\omega t)) - \frac{\kappa q^2}{4a}\cot(\omega t)(\frac{a}{a(t)} - 1)$.

(ii) Using the relation $\coth(x) \overset{x\ll 1}{=} 1/x - x/3 + \ldots$ and $1/\sinh(x) \overset{x\ll 1}{=} 1/x - x/6 + \ldots$, the high temperature expansion ($T \gg \hbar\omega$) of the density operator obtains

$$\rho(q,q') \simeq \left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2} e^{-m(q-q')^2/2\beta\hbar^2} \exp\left[-\frac{\hbar\beta m\omega^2}{6\hbar}(q^2+q'^2+qq')\right] \simeq \delta(q-q')e^{-\frac{\beta m\omega^2 q^2}{2}},$$

i.e. one recovers the classical Maxwell–Boltzmann distribution!

3. (a) Solving the Schrödinger equation, the wavefunctions obeying periodic boundary conditions take the form $\psi_n = e^{in\theta}/\sqrt{2\pi}$, n integer, and the eigenvalues are given by $E_n = n^2/2I$. Cast in the eigenbasis representation, the partition function assumes the form (3.61).

(b) Interpreted as a Feynman path integral, the quantum partition function takes the form of a propagator with

$$\mathcal{Z} = \int_0^{2\pi} d\theta\ \langle\theta|e^{-\beta\hat{H}}|\theta\rangle = \int_0^{2\pi} d\theta \int_{\theta(\beta)=\theta(0)=\theta} D\theta(\tau) \exp\left[-\int_0^\beta d\tau \frac{I}{2}\dot{\theta}^2\right].$$

The trace implies that paths $\theta(\tau)$ must start and finish at the same point. However, to accommodate the invariance of the field configuration θ under translation by 2π we must must impose the boundary conditions shown in the question.

(c) Varying the action with respect to θ we obtain the classical equation $I\ddot{\theta} = 0$. Solving this equation subject to the boundary conditions, we obtain the solution given in the question. Evaluating the Euclidean action, one finds

$$\int_0^\beta (\partial_\tau\theta)^2 d\tau \ = \ \int_0^\beta \left[\frac{2\pi m}{\beta} + \partial_\tau\eta\right]^2 d\tau = \beta\left(\frac{2\pi m}{\beta}\right)^2 + \int_0^\beta (\partial_\tau\eta)^2 d\tau.$$

Thus, one obtains the partition function (3.62), where

$$\mathcal{Z}_0 = \int D\eta(\tau) \exp\left[-\frac{I}{2}\int_0^\beta (\partial_\tau\eta)^2 d\tau\right] = \sqrt{\frac{2\pi I}{\beta}}.$$

denotes the free particle partition function. The latter can be obtained from direct evaluation of the free particle propagator.

(d) Applying the Poisson summation formula with $h(x) = \exp[-\frac{(2\pi)^2 I}{2\beta}x^2]$, one finds that

$$\sum_{m=-\infty}^{\infty} e^{-\frac{(2\pi)^2 I m^2}{2\beta}} = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\phi\, e^{-\frac{(2\pi)^2 I}{2\beta}\phi^2 + 2\pi i n\phi} = \sqrt{\frac{\beta}{2\pi I}} \sum_{n=-\infty}^{\infty} e^{-\frac{\beta}{2I}n^2}.$$

Multiplication with $\mathcal{Z}_0$ obtains the result.

4. (a) In the double well potential, the extremal field configurations of the Euclidean action involve consecutive sequences of instanton/anti–instanton pairs. However, in the periodic potential, the q instantons and q' anti–instantons can appear in any sequence provided only that $q - q' = n - m$. In this case, the Feynman amplitude takes the form

$$G(ma, na; \tau) \sim \sum_{q=0}^{\infty} \sum_{q'=0}^{\infty} \frac{\delta_{q-q',n-m}}{q!\, q'!} (\tau K e^{-S_{\text{inst.}}/\hbar})^{q+q'}$$

(b) To evaluate the instanton summation, one may make use of the identity $\delta_{q-q',n-m} = \int_0^{2\pi} e^{i(q-q'-n+m)\theta} d\theta/(2\pi)$. As a result, one obtains

$$\begin{aligned} G(ma, na; \tau) &\sim e^{\omega\tau/2} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i(n-m)\theta} \sum_{q=0}^{\infty} \frac{(\tau K e^{i\theta} e^{-S_{\text{inst.}}/\hbar})^q}{q!} \sum_{q'=0}^{\infty} \frac{(\tau K e^{-i\theta} e^{-S_{\text{inst.}}/\hbar})^{q'}}{q'!} \\ &\sim e^{\omega\tau/2} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i(n-m)\theta} \exp\left[\frac{\Delta\epsilon\tau}{\hbar} e^{i\theta}\right] \exp\left[\frac{\Delta\epsilon\tau}{\hbar} e^{-i\theta}\right] \end{aligned}$$

from which one obtains the required result.

(c) Expanded in terms of the Bloch states of the lowest band of the periodic potential $\alpha = 0$, one obtains

$$G(ma, na; \tau) = \sum_p \psi_p^*(ma) \psi_p(na) e^{-i\epsilon_p \tau/\hbar} = \sum_p |u_p(0)|^2 e^{ip(n-m)a} e^{-i\epsilon_p\tau/\hbar}$$

Interpreting $\theta = pa$, and taking $|u_p(0)|^2 =$ const. independent of p, one can draw the correspondence $\epsilon_p = \hbar\omega/2 - 2\Delta\epsilon \cos(pa)$.

4.4 Questions on the Field Integral Method

1. **Exercises on Fermion Coherent States:** To practice the coherent state method, we begin with a few simple exercises on the fermionic coherent state which complements the structures discussed in the main text.

   Considering a fermionic coherent state $|\eta\rangle$, verify the following identities: (a) $\langle\eta|a_i^\dagger = \langle\eta|\bar{\eta}_i$, (b) $a_i^\dagger|\eta\rangle = -\partial_{\eta_i}|\eta\rangle$ and $\langle\eta|a_i = \partial_{\bar{\eta}_i}\langle\eta|$, (c) $\langle\eta|\nu\rangle = \exp[\sum_i \bar{\eta}_i\nu_i]$, and (d) $\int d(\bar{\eta},\eta)\, d\eta_i\; e^{-\sum_i \bar{\eta}_i\eta_i}|\eta\rangle\langle\eta| = \mathbf{1}_{\mathcal{F}}$, where $d(\bar{\eta},\eta) \equiv \prod_i d\bar{\eta}_i d\eta_i$. Finally, (e) show that $\langle n|\psi\rangle\langle\psi|n\rangle = \langle\zeta\psi|n\rangle\langle n|\psi\rangle$, where $|n\rangle$ is an n-particle state in Fock space while $|\psi\rangle$ is a coherent state.

2. **Feynman path integral from the Functional Field Integral**

   The abstraction of the coherent state representation betrays the close similarity between the Feynman and coherent state path integrals. To help elucidate the connection, the goal of the present problem is to confirm that the Feynman path integral of the quantum harmonic oscillator follows from the coherent state path integral.

   Consider the simplest bosonic many-body Hamiltonian, $\hat{H} = \hbar\omega(a^\dagger a + \frac{1}{2})$, where $a^\dagger$ creates 'structureless' particles, i.e. states in a one–dimensional Hilbert space. $\hat{H}$ can be interpreted as the Hamiltonian of a single oscillator degree of freedom. Show that the field integral for the partition function $\mathcal{Z} = \mathrm{tr}\,[\exp(-\beta\hat{H})]$ can be mapped onto the (imaginary–time) path integral of an harmonic oscillator by a suitable variable transformation. [Hint: Let yourself be guided by the fact that the conjugate operator pair $(a, a^\dagger)$ is related to the momentum and coordinate operators $(\hat{p}, \hat{q})$ through a canonical transformation.]

3. **Quantum Partition Function of the Harmonic Oscillator** The following involves a practice exercise on elementary field integral manipulations, and infinite products.

   Compute the partition function of the harmonic oscillator Hamiltonian in the field integral formulation. To evaluate the resulting infinite product over Matsubara frequencies apply the formula $x/\sin x = \prod_{n=1}^{\infty}(1 - x^2/(\pi n)^2)^{-1}$. [Hint: The normalization of the result can be fixed by demanding that, in the zero temperature limit, the oscillator occupies its ground state.] Finally, compute the partition function by elementary means and check your result. As an additional exercise, repeat the same steps for the 'fermionic oscillator', i.e. with $a, a^\dagger$ fermion operators. Here you will need the auxiliary identity $\cos x = \prod_{n=1}^{\infty}(1 - \frac{x^2}{(\pi(n+1/2))^2})$.

4.5 Answers

1. Making use of the rules of Grassmann algebra,

(a) $$\langle\eta|a_i^\dagger = \langle 0|\exp[-\sum_j a_j\bar\eta_j]a_i^\dagger = \langle 0|\prod_j(1-a_j\bar\eta_j)a_i^\dagger = \langle 0|(1-a_i\bar\eta_i)a_i^\dagger\prod_{j\neq i}(1-a_j\bar\eta_j)$$
$$= \underbrace{\langle 0|a_ia_i^\dagger}_{=\langle 0|[a_i,a_i^\dagger]_+=\langle 0|}\bar\eta_i\prod_{j\neq i}(1-a_j\bar\eta_j) = \langle 0|\prod_j(1-a_j\bar\eta_j)\bar\eta_i = \langle\eta|\bar\eta_i\,,$$

(b) $$a_i^\dagger|\eta\rangle = \underbrace{a_i^\dagger(1-\eta_ia_i^\dagger)}_{=a_i^\dagger=\partial_{\eta_i}\eta_ia_i^\dagger=-\partial_{\eta_i}(1-\eta_ia_i^\dagger)}\prod_{j\neq i}(1-\eta_ja_j^\dagger)|0\rangle = -\partial_{\eta_i}\prod_j(1-\eta_ja_j^\dagger)|0\rangle = -\partial_{\eta_i}|\eta\rangle\,,$$
$$\langle\eta|a_i = \langle 0|\prod_{j\neq i}(1-a_j\bar\eta_j)\underbrace{(1-a_i\bar\eta_i)a_i}_{=a_i=-\partial_{\bar\eta_i}a_i\bar\eta_i=\partial_{\bar\eta_i}(1-a_i\bar\eta_i)} = \partial_{\bar\eta_i}\langle 0|\prod_j(1-a_j\bar\eta_j) = \partial_{\bar\eta_i}\langle\eta|\,,$$

(c) $$\langle\eta|\nu\rangle = \langle\eta|\prod_i\underbrace{(1-\nu_ia_i^\dagger)}_{(1+a_i^\dagger\nu_i)}|0\rangle = \langle\eta|\prod_i\underbrace{(1+\bar\eta_i\nu_i)}_{\exp[\sum_i\bar\eta_i\nu_i]}|0\rangle = \exp[\sum_i\bar\eta_i\nu_i]\,.$$

(d) To prove the completeness of fermion coherent states, we apply Schur's lemma, i.e. we need to show that $[a_j^{(\dagger)}, \int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta|] = 0$.

$$a_j^\dagger\int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta| = -\int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i}\partial_{\eta_j}|\eta\rangle\langle\eta|$$
$$= \int d(\bar\eta,\eta)\,\underbrace{\partial_{\eta_j}\left(e^{-\sum_i\bar\eta_i\eta_i}\right)}_{=\bar\eta_je^{-\sum_i\bar\eta_i\eta_i}}|\eta\rangle\langle\eta| = \int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta|a_j^\dagger$$

$$a_j\int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta| = \int d(\bar\eta,\eta)\quad\underbrace{e^{-\sum_i\bar\eta_i\eta_i}\eta_j}_{=-\partial_{\bar\eta_j}\left(e^{-\sum_i\bar\eta_i\eta_i}\right)}\quad|\eta\rangle\langle\eta|$$
$$= \int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\partial_{\bar\eta_j}\langle\eta| = \int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta|a_j\,.$$

The constant of proportionality is fixed by taking the expectation value with the vacuum.

$$\langle 0|\int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta|0\rangle \;=\; \int d(\bar\eta,\eta)\, e^{-\sum_i\bar\eta_i\eta_i} = 1\,.$$

(e) A general n-particle state is given as $|n\rangle = a_1^\dagger\ldots a_n^\dagger|0\rangle$, $\langle n| = \langle 0|a_n\ldots a_1$, where we neglected a normalization factor. The matrix element $\langle n|\psi\rangle$, thus, reads

$$\langle n|\psi\rangle = \langle 0|a_n\ldots a_1|\psi\rangle = \langle 0|\psi_n\ldots\psi_1|\psi\rangle = \psi_n\ldots\psi_1\,.$$

Similarly, we obtain $\langle\psi|n\rangle = \bar\psi_1\ldots\bar\psi_n$. Using these results,

$$\begin{aligned}\langle n|\psi\rangle\langle\psi|n\rangle &= \psi_n\ldots\psi_1\bar\psi_1\ldots\bar\psi_n = \psi_1\bar\psi_1\ldots\psi_n\bar\psi_n\\ &= (\zeta\bar\psi_1\psi_1)\ldots(\zeta\bar\psi_n\psi_n) = (\zeta\bar\psi_1)\ldots(\zeta\bar\psi_n)\psi_n\ldots\psi_1 = \langle-\zeta\psi|n\rangle\langle n|\psi\rangle\,.\end{aligned}$$

2. In the coherent state representation, the quantum partition function of the oscillator Hamiltonian is expressed in terms of the path integral ($\hbar = 1$)

$$\mathcal{Z} = \int D(\bar{\phi}, \phi)\ \exp\left[- \int_0^\beta d\tau \left(\bar{\phi} \partial_\tau \phi + \omega \bar{\phi} \phi \right) \right] , \tag{4.42}$$

where $\phi(\tau)$ denotes a complex scalar field, the constant factor $e^{-\beta\omega/2}$ has been absorbed into the measure of the functional integral $D(\bar{\phi}, \phi)$, and we have set the chemical potential $\mu = 0$. The connection between the coherent state and Feynman integral is established by the change of field variables, $\phi(\tau) = \left(\frac{m\omega}{2}\right)^{1/2} \left(q(\tau) + \frac{ip(\tau)}{m\omega} \right)$, where $p(\tau)$ and $q(\tau)$ represent real fields. Substituting this representation in Eq. (4.42), and rearranging some terms by integrating by parts, the connection is established: $\mathcal{Z} = \int D(p,q)\ \exp[-\int_0^\beta d\tau(-ip\dot{q} + \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2)]$.

3. Making use of the Gaussian functional integral for complex fields, one obtains from Eq. (4.42) ($\hbar = 1$)

$$\begin{aligned} \mathcal{Z}_{\rm B} &\sim \det(\partial_\tau + \omega)^{-1} \sim \prod_{\omega_n} (i\omega_n + \omega)^{-1} \sim \prod_{n=1}^{\infty} \left[\left(\frac{2n\pi}{\beta} \right)^2 + \omega^2 \right]^{-1} \\ &\sim \prod_{n=1}^{\infty} \left[1 + \left(\frac{\beta\omega}{2\pi n} \right)^2 \right]^{-1} \sim \frac{1}{\sinh(\beta\omega/2)} . \end{aligned}$$

Now, in the limit of small temperatures, the partition function is dominated by the ground state, $\lim_{\beta\to\infty} \mathcal{Z}_{\rm B} = \exp[-\beta\omega/2]$, which fixes the constant of proportionality. Thus, $\mathcal{Z}_b = [2\sinh(\beta\hbar\omega/2)]^{-1}$.

In the fermionic case, the Gaussian integration obtains a product over eigenvalues in the numerator and we have to use fermionic Matsubara frequencies, $\omega_n = (2n+1)\pi/\beta$:

$$\begin{aligned} \mathcal{Z}_f &\sim \det(\partial_\tau + \omega) \sim \prod_{\omega_n} (i\omega_n + \omega) \sim \prod_{n=1}^{\infty} \left[\left(\frac{(2n+1)\pi}{\beta} \right)^2 + \omega^2 \right] \\ &\sim \prod_{n=1}^{\infty} \left[1 + \left(\frac{\beta\omega}{(2n+1)\pi} \right)^2 \right] \sim \cosh(\beta\omega/2) . \end{aligned}$$

Fixing the normalization, one obtains $\mathcal{Z}_f = 2e^{-\beta\omega}\cosh(\beta\omega/2)$. Altogether, these results are easily confirmed by direct computation, viz.

$$\begin{aligned} \mathcal{Z}_{\rm B} &= e^{-\beta\omega/2} \sum_{n=0}^{\infty} e^{-n\beta\omega} = \frac{e^{-\beta\omega/2}}{1 - e^{-\beta\omega}} = \frac{1}{2\sinh(\beta\omega/2)} , \\ \mathcal{Z}_{\rm F} &= e^{-\beta\omega/2} \sum_{n=0}^{1} e^{-n\beta\omega} = e^{-\beta\omega/2}(1 + e^{-\beta\omega}) = 2e^{-\beta\omega}\cosh(\beta\omega/2) . \end{aligned}$$

5.5 Problem Set

5.5.1 Questions on the Functional Field Integral

1. In chapter 4., the connection between the coherent state path integral and the Feynman path integral for a Harmonic oscillator was exposed. The aim of this problem is to extend this calculation to obtain the Lagrangian form of the path integral for a harmonic chain from the coherent state path integral. In chapter 1 we derived a free scalar field theory for the classical Harmonic chain. Qauntising the classical theory, we showed that, in second quantised form, the Hamiltonian was given by

$$\hat{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right),$$

where $\omega_k = k_s a^2 k^2/m$. Absorbing the zero-point energy into the definition of the functional integral measure $D[\bar{\psi}_k, \psi_k]$, the corresponding coherent state path integral for the quantum partition function assumes the form

$$\mathcal{Z} = \int D[\bar{\psi}_k, \psi_k] \exp\left[- \int_0^\beta d\tau \sum_k \left(\bar{\psi}_k \partial_\tau \psi_k + \hbar\omega_k \bar{\psi}_k \psi_k \right) \right],$$

where $\psi_k(\tau)$ denotes a complex scalar field, and the chemical potential has been set to zero $\mu = 0$.

(a) By applying the change of field variables,

$$\psi_k(\tau) = \left(\frac{m\omega_k}{2\hbar} \right)^{1/2} \left[q_k(\tau) + \frac{i p_k(\tau)}{m\omega_k} \right]$$

where we choose $\bar{q}_k(\tau) = q_{-k}(\tau)$ and $\bar{p}_k(\tau) = p_{-k}(\tau)$, show that the path integral can be cast in the Hamiltonian form of the Feynman path integral.

(b) Integrating over the fields $p_k(\tau)$, obtain the Lagrangian form of the path integral for the quantum partition function. Returning to the real space representation, show that the corresponding effective action takes the form

$$\mathcal{Z} = \int Dq(x) \exp\left[- \int_0^\beta d\tau \int_0^L dx \left(\frac{1}{2} m\dot{q}^2 + \frac{1}{2} k_s a^2 (\partial_x q)^2 \right) \right].$$

---

2. **Zero temperature gap equation**: In our analysis of the field theory of the superconductor, by taking the order parameter Δ to be small, we restricted the validity of the field theory to vicinity of the critical temperature T_c. However, at zero temperature, we can obtain an estimate of the magnitude of the order parameter without resort to perturbative expansion.

In the mean-field approximation, i.e. taking Δ constant in space and time, show that the effective action for the BCS superconductor at *zero temperature* can be expressed in the form,[22]

$$\frac{S}{\beta L^d} = -\int \frac{d^3k}{(2\pi)^3}\int \frac{d\omega}{2\pi}\,\mathrm{tr}\ln\begin{pmatrix} -i\omega+\epsilon_{\mathbf{k}}-\mu & \Delta \\ \Delta^* & -i\omega-\epsilon_{\mathbf{k}}+\mu\end{pmatrix} + \frac{|\Delta|^2}{g}.$$

Setting $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, show that the action can be rewritten as

$$\frac{S}{\beta L^d} \simeq -\nu(\mu)\int d\xi \int \frac{d\omega}{2\pi}\ln\left(\omega^2 + |\Delta|^2 + \xi^2\right) + \frac{|\Delta|^2}{g}.$$

where $\nu(\mu)$ denotes the density of states at the Fermi level. Minimising the action with respect to Δ, obtain an expression for the gap equation. For $\omega_D \gg |\Delta|$, where ω_D denotes the Debye frequency cut-off on the ω integral, show that

$$|\Delta| = 2\omega_D \exp\left[-\frac{1}{g\nu(\mu)}\right].$$

---

3. **Mean-Field Theory of the BCS Hamiltonian**: This question involves the investigation of the BCS Hamiltonian within the so-called mean-field approximation. It is also serves as useful revision of methods of second quantisation.

   In the mean-field approximation, the microscopic Bogoluibov Hamiltonian can be expressed in second quantised form

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}}\left[\sum_{\sigma}\xi_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} - \left(\Delta^* c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} + \Delta c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\right)\right] + \frac{|\Delta|^2}{g},$$

   where $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$ and the complex order parameter is uniform and taken to be determined self-consistently as $\Delta = g\sum_{\mathbf{k}}\langle \text{g.s.}|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|\text{g.s.}\rangle$ and $\Delta^* = g\sum_{\mathbf{k}}\langle \text{g.s.}|c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}|\text{g.s.}\rangle$. In the **Nambu spinor representation**

$$\Psi^\dagger_{\mathbf{k}} = \begin{pmatrix} c^\dagger_{\mathbf{k}\uparrow} & c_{-\mathbf{k}\downarrow}\end{pmatrix}, \qquad \Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow}\end{pmatrix},$$

   the Hamiltonian can be recast in the form

$$\hat{H} = \sum_{\mathbf{k}}\left[\Psi^\dagger_{\mathbf{k}}\begin{pmatrix}\xi_{\mathbf{k}} & -\Delta \\ -\Delta^* & -\xi_{\mathbf{k}}\end{pmatrix}\Psi_{\mathbf{k}} + \xi_{\mathbf{k}}\right] + \frac{|\Delta|^2}{g}.$$

   (a) *Taking the order parameter Δ to be real*, show that the quadratic Hamiltonian can be diagonalised by a *unitary* transformation and gives

$$\hat{H} = \sum_{\mathbf{k}\sigma}\lambda_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma} + \sum_{\mathbf{k}}(\xi_{\mathbf{k}} - \lambda_k) + \frac{\Delta^2}{g},$$

[22] Note that $\frac{1}{L^d}\sum_{\mathbf{k}} \overset{L\to\infty}{=} \int \frac{d^dk}{(2\pi)^d}$ and $\frac{1}{\beta}\sum_{\omega_m} \overset{\beta\to\infty}{=} \int \frac{d\omega}{2\pi}$

where

$$\begin{pmatrix} \alpha^\dagger_{\mathbf{k}\uparrow} \\ \alpha_{-\mathbf{k}\downarrow} \end{pmatrix} = \begin{pmatrix} \cos\theta_{\mathbf{k}} & \sin\theta_{\mathbf{k}} \\ \sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c^\dagger_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow} \end{pmatrix}$$

and $\lambda_{\mathbf{k}} = (\xi^2_{\mathbf{k}} + \Delta^2)^{1/2}$.

The elementary excitations of the superconducting system are known as **Bogoluibons** and are created by the operators $\alpha^\dagger_{\mathbf{k}\uparrow}$ and $\alpha^\dagger_{-\mathbf{k}\downarrow}$. The result above show that the quasi-particles have a minimum energy gap of Δ.

(b) In terms of quasi-particle operators, the ground state of the system can be written in the form $|\text{g.s.}\rangle = \prod_{\mathbf{k}} \alpha_{\mathbf{k}\uparrow}\alpha_{-\mathbf{k}\downarrow}|\Omega\rangle$, where $|\Omega\rangle$ represents the vacuum state — i.e. $|\text{g.s.}\rangle$ is annihilated by all quasi-particle operators $\alpha_{\mathbf{k}\uparrow}$ and $\alpha_{-\mathbf{k}\downarrow}$. Expanding, show that, up to a constant factor,

$$|\text{g.s.}\rangle = \prod_{\mathbf{k}} \alpha_{-\mathbf{k}\downarrow}\alpha_{\mathbf{k}\uparrow}|\Omega\rangle \sim \prod_{\mathbf{k}} \left(\cos\theta_{\mathbf{k}} - \sin\theta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\right)|\Omega\rangle.$$

With this choice, confirm that this state is normalised. Obtain an expression for the ground state energy.

(c) Expanding the bare electron operators in terms of the quasi-particle operators, or Bogoluibons, show that the self-consistency equation $\Delta = g\sum_{\mathbf{k}}\langle\text{g.s.}|c_{\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|\text{g.s.}\rangle$ results in a self-consistent equation for Δ — the BCS Gap equation.

5.5.2 Answers

1. (a) Substituting the change of field variables, and rearranging some terms by integrating by parts, one obtains

$$\mathcal{Z} = \int D(p_k, q_k) \exp\left[- \int_0^\beta d\tau \sum_k \left(\frac{p_k p_{-k}}{2m} + \frac{1}{2} m\omega^2 q_k q_{-k} - \frac{i}{\hbar} p_{-k} \partial_\tau q_k \right) \right].$$

With the change of variables $\tau = it/\hbar$, one obtains the Hamiltonian formulation of the path integral.

(b) Performing the Gaussian integral over the fields p_k, one obtains

$$\mathcal{Z} = \int Dq_k \exp\left[- \int_0^\beta d\tau \sum_k \left(\frac{1}{2\hbar^2} m|\dot{q}_k|^2 + \frac{1}{2} m\omega_k^2 |q_k|^2 \right) \right].$$

With $\omega_k^2 = k^2 k_s a^2/m$, turning to the real space representation, one obtains the required result.

---

2. Starting with the expression for the action given in the question, differentiating S with respect to Δ one obtains

$$\frac{1}{\beta L^3} \frac{dS}{d\Delta} = -\nu(\mu) \int d\xi \int \frac{d\omega}{2\pi} \frac{\Delta^*}{\omega^2 + |\Delta|^2 + \xi^2} + \frac{\Delta^*}{g}.$$

Although the integral is formally divergent, recalling that the microscopic mechanism derives from the phonon-mediated interaction, we introduce a high energy cut-off at the Debye frequency, ω_D. As a result one obtains

$$\begin{aligned} \frac{1}{\beta L^3} \frac{dS}{d\Delta} &= -\frac{\nu(\mu)}{2} \int_{-\omega_D}^{\omega_D} \frac{\Delta^* d\xi}{(\xi^2 + |\Delta|^2)^{1/2}} + \frac{\Delta^*}{g} = -\nu(\mu)\Delta^* \sinh^{-1}\left(\frac{\omega_D}{|\Delta|} \right) + \frac{\Delta^*}{g} \\ &\simeq -\Delta^* \left[\nu(\mu) \ln\left(\frac{\omega_D}{|\Delta|} \right) - \frac{1}{g} \right]. \end{aligned}$$

Setting $dS/d\Delta = 0$, we obtain the zero temperature gap equation.

---

3. (a) Defining the unitary transformation,

$$\begin{pmatrix} \alpha^\dagger_{\mathbf{k}\uparrow} \\ \alpha_{-\mathbf{k}\uparrow} \end{pmatrix} = \begin{pmatrix} \cos\theta_{\mathbf{k}} & \sin\theta_{\mathbf{k}} \\ \sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c^\dagger_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow} \end{pmatrix},$$

the quadratic Hamiltonian is diagonalised when $\tan(2\theta_{\mathbf{k}}) = -\Delta/\xi_{\mathbf{k}}$

(b) Taking the definition from the question

$$\begin{aligned}\langle \text{g.s.}|\text{g.s.}\rangle &= \langle\Omega|\prod_{\mathbf{k}}(\cos\theta_{\mathbf{k}} - \sin\theta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow})(\cos\theta_{\mathbf{k}} - \sin\theta_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow})|\Omega\rangle \\ &= \prod_{\mathbf{k}}\left(\cos^2\theta_{\mathbf{k}} + \sin^2\theta_{\mathbf{k}}\right)\langle\Omega|\Omega\rangle.\end{aligned}$$

The corresponding ground state energy is given by

$$\langle \text{g.s.}|\hat{H}|\text{g.s.}\rangle = \sum_{\mathbf{k}}(\xi_{\mathbf{k}} - \lambda_{\mathbf{k}}) + \frac{\Delta^2}{g}.$$

(c) Making use of the relation between the bare electron operators and the quasi-particle operators, the self-consistency equation yields

$$\begin{aligned}\Delta &= \left\langle\Omega\left|\left(\cos\theta_{\mathbf{k}} - \sin\theta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\right) c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\left(\cos\theta_{\mathbf{k}} - \sin\theta_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow}\right)\right|\Omega\right\rangle \\ &= -g\sum_{\mathbf{k}}\sin\theta_{\mathbf{k}}\cos\theta_{\mathbf{k}} = \frac{g}{2}\sum_{\mathbf{k}}\frac{\Delta}{(\Delta^2+\xi^2_{\mathbf{k}})^{1/2}} \\ &\simeq \frac{g\Delta}{2}\nu(\mu)\int_{-\omega_D}^{\omega_D}\frac{d\xi}{(\Delta^2+\xi^2)^{1/2}}.\end{aligned}$$

From this result we obtain

$$g\nu(\mu)\ln\left(\frac{2\omega_D}{\Delta}\right) = 1, \qquad \Delta = 2\omega_D\exp\left[-\frac{1}{g\nu(\mu)}\right].$$

Concepts in Theoretical Physics

Concepts in Theoretical Physics

- Aim of course: to develop methods of many-body & (low-energy) quantum field theory motivated by applications!
- Synopsis
- Relation to QFT & other Part III courses?
- Prerequistes? (TPs etc.)
- Lecture notes, problem sets & books

  course web-page:
  `http://www.tcm.phy.cam.ac.uk/~bds10/`
- Supervisions

Ben Simons
Room 518 (Mott)
e-mail: bds10@cam.ac.uk

How can we develop a Quantum Theory of "Dense" Matter?

the "quantum many-body problem"...

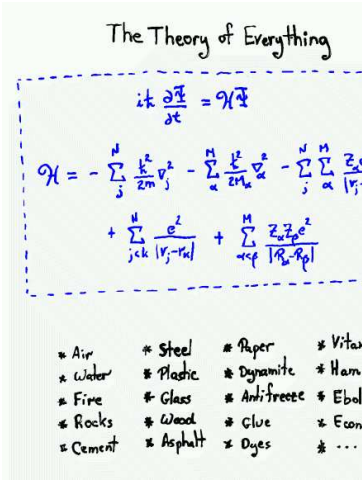
- **First principles?**

according to some,
we already have a **Theory of Everything**...

...but clearly the ability to reduce everything to simple fundamental laws does not imply the ability to start form those laws and reconstruct the universe!

- **Perturbation theory about non-interacting** (i.e. free-particle) **reference state?**

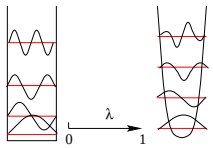
effective, but limited in scope...
consider effect of interactions...



Robert Laughlin (Nob

How do particle interactions influence properties of quantum many-particle system?

- **Non-interacting system** ⇝ ideal gas laws
  e.g. free electron theory, Debye theory, etc.
- **Weak interaction**
  ...relies on principle of "adiabatic continuity":

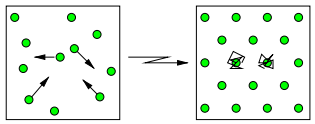


labels of wavefunctions (quantum nos.)[1]
more robust than wavefunctions themselves

⇝ "quasi-particle correspondence"...

[1] ...which depend only on fundamental symmetries (translation, rotation, etc.) and dimensionality

How do particle interactions influence properties of quantum many-particle system?



- **Strong interaction** ⇝ symmetry breaking
  (i.e. transitions to new phases of matter)

e.g. crystal, magnet, superfluid...

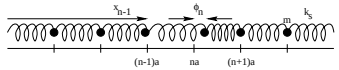
each phase characterised by
new "collective excitations"[2]

e.g. ...

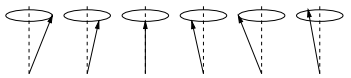
[2] i.e. particle-like excitations involving the collective motion of many elementary particles

Broken symmetry & collective modes

I. **Crystal**: broken translational symmetry
⇝ lattice vibrations (phonons)



II. **Magnet**: broken spin rotational symmetry
⇝ spin waves (magnons)



III. **Superfluid** — broken gauge symmetry
⇝ phase mode

IV. **Quark plasma** — strong interaction
broken gauge symmetry ⇝ hadrons

etc., etc.

...properties of collective excitations usually very different from elementary bare particles

Heirarchical view of matter

- Each phase of matter characterised and classified by fundamental sy

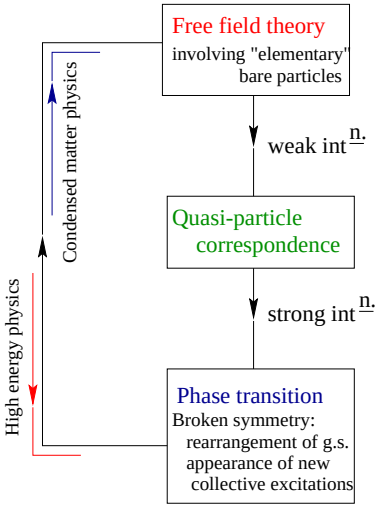
  e.g. translation, rotation, spin, gauge,...
- Within each phase, fluctuations charac (particle-like) excitations, quasi-particle properties mirror those of the free theory

  e.g. electron/hole quasi-particles,...
- Transitions between phases signalled by breaking ⇝ new collective quasi-particle e (usually very different from the elemer particles)

  e.g. fractional quantum Hall liquid,...

This heirarchy lends itself to the common language of quantum fiel

[1] ...familiar from high energy physics



Quantum Theory of Matter

I. **Microscopic Theory**

(a) Many-particle Hamiltonian...
encodes fundamental particle interactions

(b) ...cast as quantum field theory
via quantum path or field integral

(c) Mean-field theory
broken symmetries $\rightsquigarrow$ global phase structure

(d) Low-energy fluctuations
$\rightsquigarrow$ quantum field theory of collective excitations

II. **Phenomenology**

Fundamental symmetries:
constrain low-energy effective field theory

i.e. Universality!

Aim of Course

...to develop basic theoretical machinery
to address quantum many-body physics:

- Method of second quantisation:
language of many-particle quantum mechanics

- Functional field integral methods
  (a) Feynman path integral
  (b) Coherent state path integral

- [Critical phenomena
& methods of statistical field theory]

Synopsis

- Collective excitations — from particles to fie
harmonic chain & free scalar field theory; classic
modes, phonons; quantising the classical field;
analysis

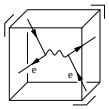
- Method of second quantisation: creation
applications to phonons, Mott-Hubbard transition
magnetism; spin wave theory; †antiferromagnetis
interacting Bose gas

- Functional methods: Feynman path integral;
integration & saddle-point analyses; semi-classic
mechanics; single & double well, instantons &
applications to soft matter & quantum friction.

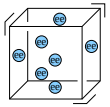
- Functional field theory: *Grassmann Algebra*; col
path integral; quantum partition function; Coope
& BCS theory; Ginzburg-Landau & statistical f
Gauge theory, Higgs mechanism & superconductiv

- Relativistic quantum mechanics: symmetries &
Klein-Gordon & Dirac equation; free particle; Kl
antiparticles; spin; coupling to classical EM field
interactions & gauge theories.

Superconductivity: A Quantum Phase Transition of the Electron Gas



▷ Exchange of lattice vibrations (phonons) between electrons
$\rightsquigarrow$ (non-local) pairing interaction

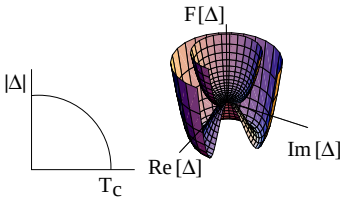


▷ At low T, electrons "condense" in pairs
cf. Bose-Einstein condensation

▷ Phase transition signalled by development of order parameter:

$$\langle \psi_\uparrow \psi_\downarrow \rangle = \Delta \equiv |\Delta| e^{i\phi}$$

possessing both amplitude & phase



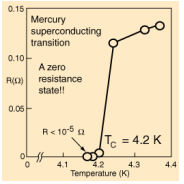
▷ Breaking of (gauge) symmetry...
(cf. ferromagnet, crystal, etc.)

...accompanied by low-energy collective phase fluctuations
(cf. spin waves, phonons, etc.)

▷ Interaction of phase field ϕ with EM-field
$\rightsquigarrow$ photon mass(!) & superconductivity
(cf. Higgs mechanism in electroweak theory)

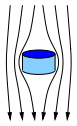
Consequences

▷ Superconductivity:



H. K. Onnes, Commun. Phys. Lab. **12**, 120 (1911)

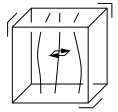
▷ Meissner Effect:

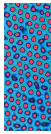


perfect diamagnetic response $\rightsquigarrow$ exclusion of magnetic field

Topological Excitations

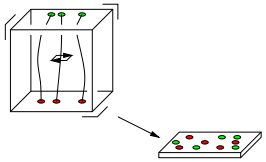
▷ Topological defects: vortices (cf. dislocations)





Vortex lattice

▷ Topological Phase Transition in Thin-films

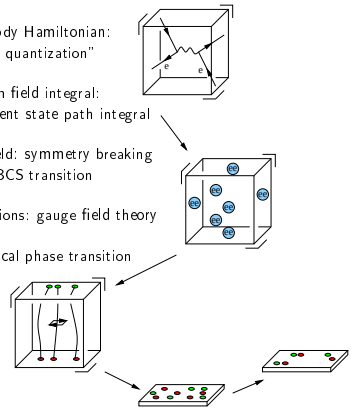


vortex plasma

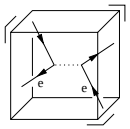
(cf.

From Microscopics to Quantum Fields

1. Many-body Hamiltonian: "second quantization"
2. Quantum field integral: coherent state path integral
3. Mean-field: symmetry breaking & BCS transition
4. Fluctuations: gauge field theory
5. Topological phase transition



Coulomb Interaction



▷ Electronic Phases of Matter:

Landau Fermi-liquid
Wigner crystal
Mott Insulator
Quantum magnetism & spin liquids
Quantum Hall fluids
Heavy fermion superconductor
Luttinger liquid
Exciton insulator & condensate

Books

▷ **Quantum Many-body theory**

*R. P. Feynman, *Statistical Mechanics*, Benjamin, New York, (1972).

N. Nagaosa, *Quantum Field Theory in Condensed Matter Physics*, Sringer 1999.

*J. W. Negele and H. Orland, *Quantum Many-Particle Systems*, Addison-Wesley Publishing, 1988.

▷ **Functional Field Integral methods**

*A. Das, *Field Theory: A Path Integral Approach*, World Scientific Publishing, (1993).

R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill, New York, (1965).

*L. S. Schulman, *Techniques and Applications of Path Integration*, John Wiley & Sons, 1981.

▷ **Relativistic Quantum Mechanics**

J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics*, McGraw-Hill (1964).

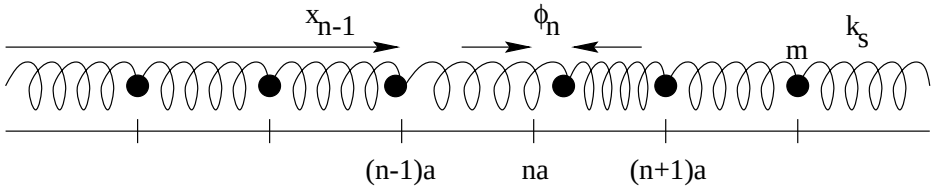
*L. H. Ryder, *Quantum Field Theory*, Cambridge University Press, 1996.

Lecture II: Collective Excitations: From Particles to Fields

Free Scalar Field Theory: Phonons

The aim of this course is to develop the machinery to explore the properties of quantum systems with very large or infinite numbers of degrees of freedom. To represent such systems it is convenient to abandon the language of individual elementary particles and speak about quantum fields. In this lecture, we will consider the simplest physical example of a free or non-interacting many-particle theory theory which will exemplify the language of classical and quantum fields. Our starting point is a toy model of a mechanical system describing a classical chain of atoms coupled by springs.

▷ Discrete elastic chain



Equilibrium position $\bar{x}_n \equiv na$; natural length a; spring constant k_s

Goal: to construct and quantise a classical field theory
for the collective (longitudinal) vibrational modes of the chain

▷ Discrete Classical Lagrangian:

$$L = T - V = \sum_{n=1}^{N} \Big(\overbrace{\frac{m}{2}\dot{x}_n^2}^{\text{k.e.}} - \overbrace{\frac{k_s}{2}(x_{n+1} - x_n - a)^2}^{\text{p.e. in spring}} \Big)$$

assume periodic boundary conditions (p.b.c.) $x_{N+1} = Na + x_1$ (and set $\dot{x}_n \equiv \partial_t x_n$)

Using displacement from equilibrium $\phi_n = x_n - \bar{x}_n$

$$L = \sum_{n=1}^{N} \left(\frac{m}{2}\dot{\phi}_n^2 - \frac{k_s}{2}\left(\phi_{n+1} - \phi_n\right)^2 \right), \qquad \text{p.b.c}: \quad \phi_{N+1} \equiv \phi_1$$

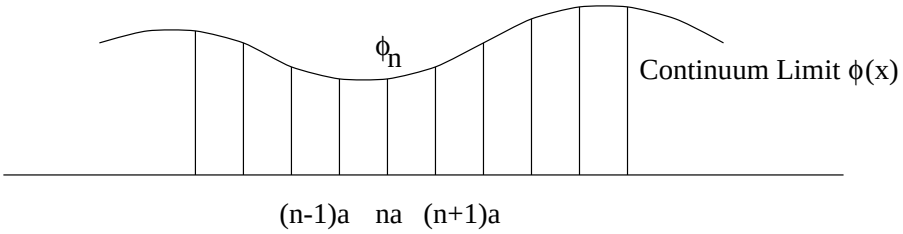
In principle, one can obtain exact solution of discrete equation of motion — see PS I

However, typically, one is not concerned with behaviour on 'atomic' scales:

1. for such purposes, modelling is too primitive!
   anharmonic contributions
2. such properties are in any case 'non-universal'

Aim here is to describe low-energy collective behaviour — generic, i.e. <u>universal</u>

In this case, it is often permissible to neglect the discreteness of the microscopic entities of the system and to describe it in terms of effective continuum degrees of freedom.



▷ Continuum Lagrangian

Describe ϕ_n as a smooth function $\phi(x)$ of a continuous variable x;
makes sense if $\phi_{n+1} - \phi_n \ll a$ (i.e. gradients small)

$$\phi_n \to a^{1/2}\phi(x)\Big|_{x=na}, \qquad \phi_{n+1} - \phi_n \to a^{3/2}\partial_x\phi(x)\Big|_{x=na}, \qquad \sum_n \longrightarrow \frac{1}{a}\int_0^{L=Na} dx$$

N.B. $[\phi(x)] = L^{1/2}$

$$\overbrace{L[\phi] = \int_0^L dx\ \mathcal{L}(\phi, \partial_x\phi, \dot{\phi})}^{\text{Lagrangian functional}}, \qquad \overbrace{\mathcal{L}(\phi, \partial_x\phi, \dot{\phi}) = \frac{m}{2}\dot{\phi}^2 - \frac{k_s a^2}{2}(\partial_x\phi)^2}^{\text{Lagrangian density}}$$

N.B. $[\mathcal{L}]$ = [energy]/[length]

▷ Classical action

$$\boxed{S[\phi] = \int dt\ L[\phi] = \int dt \int_0^L dx\ \mathcal{L}(\phi, \partial_x\phi, \dot{\phi})}$$

- N-point particle degrees of freedom $\mapsto$ continuous classical field $\phi(x)$
- Dynamics of $\phi(x)$ specified by functionals $L[\phi]$ and $S[\phi]$

What are the corresponding equations of motion...?

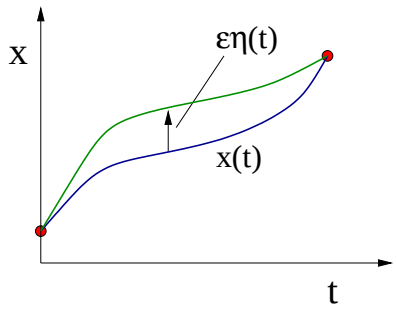
▷ Hamilton's Extremal Principle (HEP): (Revision)

Suppose classical point particle $x(t)$ described by action $S[x] = \int dt\ L(x, \dot{x})$

HEP: configurations $x(t)$ that are realised are those that extremise the action
i.e. for any smooth function $\eta(t)$, the "variation"

$$\delta S[x] \equiv \lim_{\epsilon \to 0} \frac{1}{\epsilon}(S[x + \epsilon\eta] - S[x]) = 0$$

to 1st order in ϵ, action must by stationary



Extremal condition $\mapsto$ Euler-Lagrange equations of motion

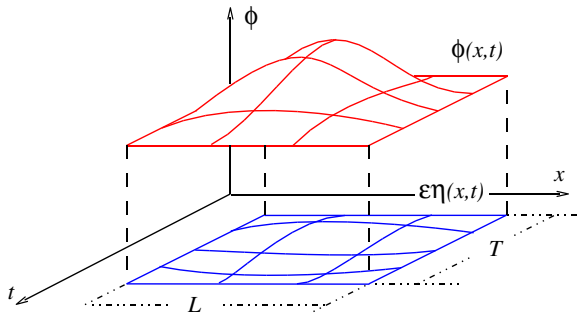
$$S[x+\epsilon\eta] = \int_0^t dt\, L(x+\epsilon\eta, \dot{x}+\epsilon\dot{\eta}) = \int_0^t dt\, (L(x,\dot{x}) + \epsilon\eta\partial_x L + \epsilon\dot{\eta}\partial_{\dot{x}} L) + O(\epsilon^2)$$

$$\delta S[x] = \int dt\, (\eta\partial_x L + \dot{\eta}\partial_{\dot{x}} L) \overset{\text{by parts}}{=} \int dt\, \overbrace{\left(\partial_x L - \frac{d}{dt}(\partial_{\dot{x}} L)\right)}^{=0} \eta = 0$$

Note: boundary terms vanish by construction

(The variation $\dfrac{\delta L}{\delta x} = \partial_x L - \dfrac{d}{dt}(\partial_{\dot{x}} L)$ is an example of functional differentiation.
A formal discussion of its legitimacy is included in the lecture notes.)

How does HEP generalise to continuum field $x \mapsto \phi(x)$?



Apply same extremal principle: $\phi(x,t) \mapsto \phi(x,t) + \epsilon\eta(x,t)$
with both ϕ and η both periodic in x

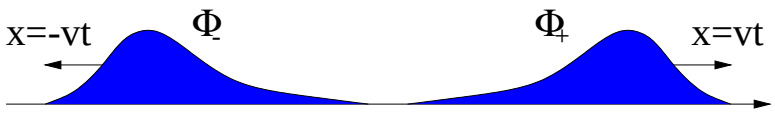
$$S[\phi+\epsilon\eta] = S[\phi] + \epsilon \int_0^t dt \int_0^L dx \left(m\dot{\phi}\dot{\eta} - k_s a^2 \partial_x\phi\partial_x\eta\right) + O(\epsilon^2).$$

Integrating by parts *boundary terms vanish by construction:* $\eta\dot{\phi}|_0^t = 0 = \eta\partial_x\phi|_0^L$

$$\delta S = -\int_0^t dt \int_0^L dx \left(m\ddot{\phi} - k_s a^2 \partial_x^2\phi\right)\eta = 0$$

Since $\eta(x,t)$ is an arbitrary smooth function, we must have

$$\left(m\partial_t^2 - k_s a^2 \partial_x^2\right)\phi = 0$$



i.e. $\phi(x,t)$ obeys classical wave equation

General solutions are of the form: $\phi_+(x+vt) + \phi_-(x-vt)$
where $v = a\sqrt{k_s/m}$ is sound wave velocity and $\phi_\pm$ are arbitrary smooth functions

More generally, for the Lagrangian density $\mathcal{L} = \mathcal{L}(\phi, \partial_x\phi, \dot{\phi})$,

$$\frac{\partial \mathcal{L}}{\partial \phi} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\phi}} - \frac{d}{dx}\frac{\partial \mathcal{L}}{\partial(\partial_x \phi)} = 0$$

▷ COMMENTS

- Low-energy collective excitations — known as phonons — are lattice vibrations
  propagating as sound waves to left or right at constant velocity v

- Trivial behaviour of model is a direct consequence of its simplistic definition:
  Lagrangian is quadratic in fields $\mapsto$ linear equation of motion
  Higher order couplings (i.e. interactions) $\mapsto$ dissipation and dispersion

- L is said to be a 'free (i.e. non-interacting) scalar (i.e. one-component) field theory'

- In higher dimensions, field has vector components
  $\mapsto$ transverse and longintudinal modes

Variational principle is example of FUNCTIONAL ANALYSIS — a useful (but not essential
concept for this course) — see lecture notes

Lecture III: Quantising the Classical Field

Having established that the low energy properties of the atomic chain are represented by a free scalar classical field theory, we now turn to the formulation of the quantum system.

▷ Canonical Quantisation procedure: recall point particle mechanics

1. Define canonical momentum $p = \partial_{\dot{x}} L$
2. Construct Hamiltonian $H = p\dot{x} - L(p, x)$
3. Promote position and momentum to operators with canonical commutation relations

$$x \mapsto \hat{x}, \qquad p \mapsto \hat{p}, \qquad [\hat{p}, \hat{x}] = -i\hbar, \qquad H \mapsto \hat{H}$$

1. Canonical momentum: natural generalisation to continuous field

$$\boxed{\pi(x) \equiv \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x)}}$$

applied to atomic chain, $\pi = \partial_{\dot{\phi}}(m\dot{\phi}^2/2) = m\dot{\phi}$

2. Classical Hamiltonian:

$$H[\phi, \pi] \equiv \int dx \quad \overbrace{\left[\pi\dot{\phi} - \mathcal{L}(\partial_x\phi, \dot{\phi})\right]}^{\text{Hamiltonian density } \mathcal{H}(\phi,\pi)}$$

$$\text{i.e.} \qquad \mathcal{H}(\phi, \pi) = \frac{1}{2m}\pi^2 + \frac{k_s a^2}{2}(\partial_x\phi)^2$$

3. Canonical Quantisation:

(a) promote $\phi(x)$ and $\pi(x)$ to operators: $\phi \mapsto \hat{\phi}$, $\pi \mapsto \hat{\pi}$

(b) generalise the canonical commutation relations

$$[\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar\delta(x - x')$$

N.B. $[\delta(x - x')] = [\text{Length}]^{-1}$ (exercise)

Operator-valued functions $\hat{\phi}$ and $\hat{\pi}$ referred to as quantum fields

Comments: *$\hat{H}$ represents a quantum field theoretical formulation of elastic chain, but not yet a solution. In fact, the development of a variety of methods for the analysis of quantum field theoretical models will represent major part of course. Here, objective is merely to exemplify how physical information can be extracted from this particular model.*

As with any fn, operator-valued fns. can be expressed as Fourier series expansion:

$$\begin{Bmatrix} \hat{\phi}(x) \\ \hat{\pi}(x) \end{Bmatrix} = \frac{1}{L^{1/2}} \sum_k e^{\pm ikx} \begin{Bmatrix} \hat{\phi}_k \\ \hat{\pi}_k \end{Bmatrix}, \qquad \begin{Bmatrix} \hat{\phi}_k \\ \hat{\pi}_k \end{Bmatrix} \equiv \frac{1}{L^{1/2}} \int_0^{L=Na} dx\, e^{\mp ikx} \begin{Bmatrix} \hat{\phi}(x) \\ \hat{\pi}(x) \end{Bmatrix}$$

$\sum_k$ runs over all quantised wavevectors $k = 2\pi m/L$, $m \in \mathcal{Z}$

Exercise: confirm $[\hat{\pi}_k, \hat{\phi}_{k'}] = -i\hbar\delta_{kk'}$

Advice: *Maintain strict conventions(!) — we will pass freely between real and Fourier space (and we will not care to write a tilde in each case).*

Hermiticity: $\hat{\phi}^\dagger(x) = \hat{\phi}(x)$, implies $\hat{\phi}_k^\dagger = \hat{\phi}_{-k}$ (similarly $\hat{\pi}$). Using

$$\int_0^L dx\ (\partial\hat{\phi})^2 = \sum_{k,k'} (ik\hat{\phi}_k)(ik'\hat{\phi}_{k'}) \overbrace{\frac{1}{L}\int_0^L dx\, e^{i(k+k')x}}^{\delta_{k+k',0}} = \sum_k k^2 \hat{\phi}_k \hat{\phi}_{-k} \quad \left(= \sum_k k^2 |\hat{\phi}_k|^2 \right)$$

$$\hat{H} = \sum_k \Big[\frac{1}{2m}\hat{\pi}_k\hat{\pi}_{-k} + \overbrace{\frac{k_s a^2}{2}k^2}^{m\omega_k^2/2}\, \hat{\phi}_k\hat{\phi}_{-k} \Big]$$

$\omega_k = v|k|$, $v = a(k_s/m)^{1/2}$

In Fourier representation, 'modes k' decoupled

Comments:

- $\hat{H}$ provides explicit description of the low energy excitations of the system (waves) in terms of their microscopic constituents (atoms)
- However, it would be much more desirable to develop a picture where the relevant excitations appear as fundamental units...

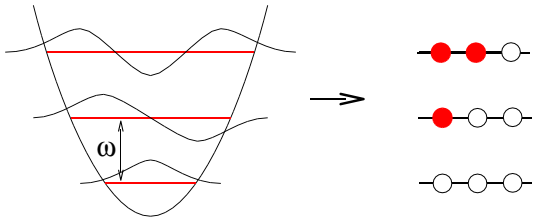
to learn how, noting the structural similarity, let us digress and discuss/revise the...

▷ Quantum Harmonic Oscillator (Revisited)

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2$$

Although a single-particle problem, its property of equidistant energy level separation, $\epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right)$ suggests alternative interpretation:

State with energy ϵ_n can be viewed as an "assembly" of n elementary, structureless (i.e. the only 'quantum number' is their energy $\hbar\omega$), bosonic particles (state can be multiply occupied) each having an energy $\hbar\omega$



▷ Formally, defining the ladder operators

$$\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), \qquad \hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$$

$\rightsquigarrow$ canonical commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$ (characteristic of bosons)

$$\boxed{\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)}$$

If we find state $|0\rangle$: $\hat{a}|0\rangle = 0 \rightsquigarrow \hat{H}|0\rangle = \frac{\hbar\omega}{2}|0\rangle$, i.e. $|0\rangle$ provides ground state

Using commutation relations, one may show $|n\rangle \equiv \dfrac{1}{(n!)^{1/2}}\,\hat{a}^{\dagger n}|0\rangle$
is (normalised) eigenstate with eigenvalue $\hbar\omega(n + \frac{1}{2})$

COMMENTS: a-representation affords a many-particle interpretation

- $|0\rangle$ represents 'vacuum', i.e. state with no particles
- $\hat{a}^\dagger|0\rangle$ represents state with a single particle of energy $\hbar\omega$
- $\hat{a}^{\dagger n}|0\rangle$ is many-body state with n particles
  i.e. $\hat{a}^\dagger$ is an operator that creates particles
- In 'diagonal' form $\hat{H} = \hbar\omega(\hat{a}^\dagger a + \frac{1}{2})$ simply counts number of particles,
  i.e. $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$, and assigns an energy $\hbar\omega$ to each

▷ Returning to quantum harmonic chain, let us then introduce new representation:

$$a_k \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_k + \frac{i}{m\omega_k}\hat{\pi}_{-k}\right), \qquad a_k^\dagger \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_{-k} - \frac{i}{m\omega_k}\hat{\pi}_k\right)$$

N.B. By convention, drop hat from operators a

with $[a_k, a_{k'}^\dagger] = \dfrac{i}{2\hbar}\Big(\overbrace{[\hat{\pi}_{-k}, \hat{\phi}_{-k'}]}^{-i\hbar\delta_{kk'}} - [\hat{\phi}_k, \hat{\pi}_{k'}]\Big) = \delta_{kk'}$

i.e. bosonic commutation relations

▷ And obtain (exercise — PS I)

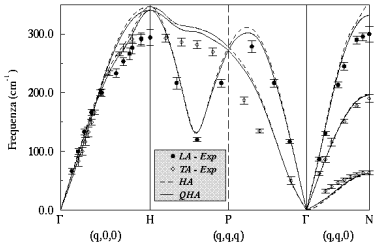
$$\boxed{\hat{H} = \sum_k \hbar\omega_k\left(a_k^\dagger a_k + \frac{1}{2}\right)}$$

Elementary collective excitations of quantum chain (phonons)
created/annihilated by bosonic operators $a_k^\dagger$ and a_k

Spectrum of excitations is linear $\omega_k = v|k|$ (cf. relativistic)

LESSONS:

- Low-energy excitations of discrete model involve slowly varying collective modes;
  i.e. each mode involves many atoms
- Low-energy ($k \to 0$) $\mapsto$ long-wavelength excitations
  — i.e. universal, insensitive to microscopic detail;
- This fact allows many different systems to be mapped onto a few (hopefully simple)
  classical field theories;
- Canonical quantisation procedure for point mechanics generalises to
  quantum field theory;
- Simplest model actions (such as the one considered here) are quadratic in the fields
  — known as free field theory;
- More generally, interactions $\rightsquigarrow$ non-linear eqs. of motion
  and interacting quantum field theories



▷ Other examples? †Quantum Electrodynamics

EM field — specified by 4-vector potential $A(x) = (\phi(x), \mathbf{A}(x))$ $(c = 1)$

Classical action : $$\boxed{S[A] = \int d^4x\ \mathcal{L}(A), \qquad \mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}}$$

$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ — EM field tensor

Classical equation of motion:

$$\overbrace{\partial_{A^\alpha}\mathcal{L} - \partial^\beta \frac{\partial \mathcal{L}}{\partial(\partial^\beta A^\alpha)} = 0}^{\text{Euler} - \text{Lagrange eqns.}} \quad \mapsto \quad \overbrace{\partial_\alpha F^{\alpha\beta} = 0}^{\text{Maxwell's eqns.}}$$

Quantisation of classical field theory identifies elementary excitations: photons

for more details, see handout, or go to QFT!

Lecture IV: Second Quantisation

We have seen how the elementary excitations of the quantum chain can be presented in terms of new elementary quasi-particles by the ladder operator formalism. Can this approach be generalised to accommodate other many-body systems? The answer is provided by the method of second quantisation — an essential tool for the development of interacting many-body field theories. The first part of this section is devoted largely to formalism — the second part to applications aimed at developing fluency.

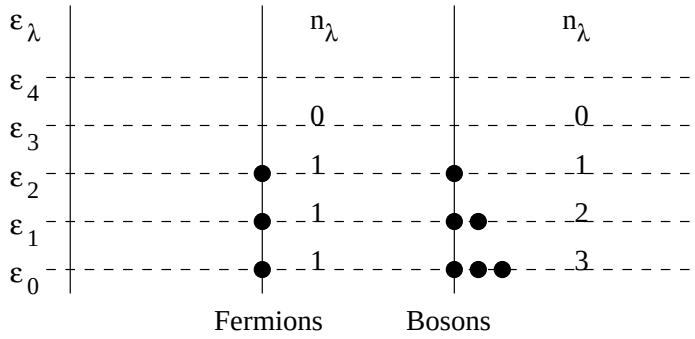
Reference: see Feynman's book on "Statistical Mechanics"

▷ Notations and Definitions

Consider a single-particle Schrodinger equation:

$$\boxed{\hat{H}|\psi_\lambda\rangle = \epsilon_\lambda|\psi_\lambda\rangle}$$

How can one construct a many-body wavefunction?
Particle indistinguishability demands symmetrisation:



e.g. two-particle wavefunction for fermions *i.e. particle 1 in state 1, particle 2...*

$$\psi_F(x_1,x_2) \equiv \frac{1}{\sqrt{2}}(\overbrace{\psi_1}^{\text{state 1}}(\overbrace{x_1}^{\text{particle 1}})\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2))$$

In Dirac notation:

$$|1,2\rangle_F \equiv \frac{1}{\sqrt{2}}\left(|\psi_1\rangle \otimes |\psi_2\rangle - |\psi_2\rangle \otimes |\psi_1\rangle\right)$$

▷ General normalised, symmetrised, N-particle wavefunction
of bosons ($\zeta = +1$) or fermions ($\zeta = -1$)

$$\boxed{|\lambda_1,\lambda_2,\ldots\lambda_N\rangle \equiv \frac{1}{\sqrt{N!\prod_{\lambda=0}^{\infty} n_\lambda!}}\sum_{\mathcal{P}} \zeta^{\mathcal{P}}|\psi_{\lambda_{\mathcal{P}1}}\rangle \otimes |\psi_{\lambda_{\mathcal{P}2}}\rangle \ldots \otimes |\psi_{\lambda_{\mathcal{P}N}}\rangle}$$

- n_λ — no. of particles in state λ
  (for fermions, Pauli exclusion: $n_\lambda = 0, 1$, i.e. $|\lambda_1,\lambda_2,\ldots\lambda_N\rangle$ is a Slater determinant)

- $\sum_{\mathcal{P}}$: Summation over $N!$ permutations of $\{\lambda_1, \ldots \lambda_N\}$
  required by particle indistinguishability
- Parity $\mathcal{P}$ — no. of transpositions of two elements which brings permutation $(\mathcal{P}_1, \mathcal{P}_2, \cdots \mathcal{P}_N)$ back to ordered sequence $(1, 2, \cdots N)$

Evidently, "first quantised" representation looks clumsy!
motivates alternative representation...

▷ Second quantisation

Define vacuum state: $|\Omega\rangle$, and set of field operators a_λ and adjoints $a_\lambda^\dagger$ — no hats!

$$\boxed{a_\lambda|\Omega\rangle = 0, \qquad \frac{1}{\sqrt{\prod_{\lambda=0}^{\infty} n_\lambda!}} \prod_{i=1}^{N} a_{\lambda_i}^\dagger |\Omega\rangle = |\lambda_1, \lambda_2, \ldots \lambda_N\rangle}$$

cf. bosonic ladder operators for phonons *N.B. ambiguity of ordering?*

Field operators fulfil commutation relations for bosons (fermions)

$$\left[a_\lambda, a_\mu^\dagger\right]_{-\zeta} = \delta_{\lambda\mu}, \qquad \left[a_\lambda, a_\mu\right]_{-\zeta} = \left[a_\lambda^\dagger, a_\mu^\dagger\right]_{-\zeta} = 0$$

where $[\hat{A}, \hat{B}]_{-\zeta} \equiv \hat{A}\hat{B} - \zeta\hat{B}\hat{A}$ is the commutator (anti-commutator)

- Operator $a_\lambda^\dagger$ creates particle in state λ, and a_λ annihilates it
- Commutation relations imply Pauli exclusion for fermions: $a_\lambda^\dagger a_\lambda^\dagger = 0$
- Any N-particle wavefunction can be generated by application of set of N operators to a unique vacuum state

$$\text{e.g.} \qquad |1, 2\rangle = a_2^\dagger a_1^\dagger |\Omega\rangle$$

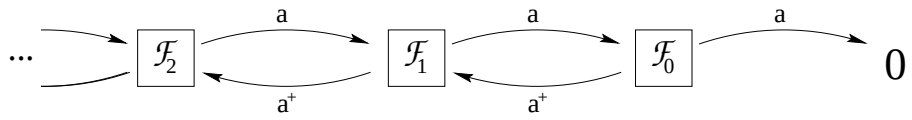
- Symmetry of wavefunction under particle interchange maintained by commutation relations of field operators

$$\text{e.g.} \qquad |1, 2\rangle = a_2^\dagger a_1^\dagger |\Omega\rangle = \zeta a_1^\dagger a_2^\dagger |\Omega\rangle$$

(So, providing one maintains a consistent ordering convention,
the nature of that convention doesn't matter)

▷ Fock space: Defining $\mathcal{F}_N$ to be 'linear span' of all N-particle states $|\lambda_1, \lambda_2, \cdots \lambda_N\rangle$
Fock space $\mathcal{F}$ is defined as 'direct sum' $\oplus_{N=0}^{\infty}\mathcal{F}_N$

- General state $|\phi\rangle$ of the Fock space is linear combination of states with any number of particles
- Note that the vacuum state $|\Omega\rangle$ (sometimes written as $|0\rangle$) is distinct from zero!



▷ Change of basis:

Using the resolution of identity $\mathbf{1} \equiv \sum_\lambda |\lambda\rangle\langle\lambda|$, we have $\overbrace{|\tilde{\lambda}\rangle}^{a^\dagger_{\tilde{\lambda}}|\Omega\rangle} = \sum_\lambda \overbrace{|\lambda\rangle}^{a^\dagger_\lambda|\Omega\rangle} \langle\lambda|\tilde{\lambda}\rangle$

$$\text{i.e.} \quad a^\dagger_{\tilde{\lambda}} = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a^\dagger_\lambda, \qquad \text{and} \quad a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda$$

E.g. Fourier representation: $a_\lambda \equiv a_k$, $a_{\tilde{\lambda}} \equiv a(x)$

$$a(x) = \sum_k \overbrace{\langle x|k\rangle}^{e^{ikx}/\sqrt{L}} a_k, \qquad a_k = \frac{1}{\sqrt{L}} \int_0^L dx\; e^{-ikx} a(x)$$

▷ Occupation number operator: $\hat{n}_\lambda = a^\dagger_\lambda a_\lambda$ measures no. of particles in state λ

e.g. (bosons)

$$a^\dagger_\lambda a_\lambda (a^\dagger_\lambda)^n|\Omega\rangle = a^\dagger_\lambda \overbrace{a_\lambda a^\dagger_\lambda}^{1 + a^\dagger_\lambda a_\lambda} (a^\dagger_\lambda)^{n-1}|\Omega\rangle = (a^\dagger_\lambda)^n|\Omega\rangle + (a^\dagger_\lambda)^2 a_\lambda (a^\dagger_\lambda)^{n-1}|\Omega\rangle = \cdots = n(a^\dagger_\lambda)^n|\Omega\rangle$$

Exercise: check for fermions

Lecture V: Second Quantised Representation of Operators

So far we have developed an operator-based formulation of many-particle states. However, for this representation to be useful, we have to understand how the action of first quantised operators on many-particle states can be formulated within the framework of the second quantisation. To do so, it is natural to look for a formulation in the diagonal basis and recall the action of the particle number operator. To begin, let us consider...

▷ One-body operators, i.e. operators which address only one particle at a time

$$\hat{\mathcal{O}}_1 = \sum_{n=1}^{N} \hat{o}_n, \qquad \text{e.g. k.e. } \hat{T} = \sum_{n=1}^{N} \frac{\hat{p}_n^2}{2m}$$

• Suppose $\hat{o}$ diagonal in orthonormal basis $|\lambda\rangle$ *e.g.* $\hat{o} = \hat{p}^2/2m$ *with* $|p\rangle$ *and* $o_p = p^2/2m$
i.e. $\hat{o} = \sum_{\lambda=0}^{\infty} |\lambda\rangle o_\lambda \langle\lambda|, \qquad o_\lambda = \langle\lambda|\hat{o}|\lambda\rangle$

$$\begin{aligned}\langle\lambda_1', \cdots \lambda_N'|\hat{\mathcal{O}}_1|\lambda_1, \cdots \lambda_N\rangle &= \left(\sum_{i=1}^{N} o_{\lambda_i}\right) \langle\lambda_1', \cdots \lambda_N'|\lambda_1, \cdots \lambda_N\rangle \\ &= \langle\lambda_1', \cdots \lambda_N'| \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda |\lambda_1, \cdots \lambda_N\rangle,\end{aligned}$$

Since this holds for any basis state, $\hat{\mathcal{O}}_1 = \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} o_\lambda a_\lambda^\dagger a_\lambda$

i.e. in diagonal representation, simply count number of particles in state λ and multipy by corresponding eigenvalue of one-body operator

Transforming to general basis (recall $a_\lambda = \sum_\nu \langle\lambda|\nu\rangle a_\nu$)

$$\boxed{\hat{\mathcal{O}}_1 = \sum_{\lambda\mu\nu} \langle\mu|\lambda\rangle o_\lambda \langle\lambda|\nu\rangle a_\mu^\dagger a_\nu = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle a_\mu^\dagger a_\nu}$$

i.e. $\hat{\mathcal{O}}_1$ scatters particle from state ν to μ with probability amplitude $\langle\mu|\hat{o}|\nu\rangle$

▷ Examples of one-body operators:

1. Total number operator: $\hat{N} = \int dx\ a^\dagger(x)a(x) = \sum_k a_k^\dagger a_k$
2. Electron spin operator: $\hat{\mathbf{S}} = \sum_{\alpha\beta} a_\alpha^\dagger \mathbf{S}_{\alpha\beta} a_\beta, \qquad \mathbf{S}_{\alpha\beta} = \langle\alpha|\hat{\mathbf{S}}|\beta\rangle = \frac{1}{2}\sigma_{\alpha\beta}$
where $\alpha = \uparrow, \downarrow$, and σ are Pauli spin matrices

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mapsto \hat{S}^z = \frac{1}{2}(n_\uparrow - n_\downarrow), \qquad \sigma_+ = \sigma_x + i\sigma_y = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \mapsto \hat{S}^+ = a_\uparrow^\dagger a_\downarrow$$

3. Free particle Hamiltonian

$$\sum_p \frac{p^2}{2m} a_p^\dagger a_p \overset{\text{Exercise}}{=} \int_0^L dx\ a^\dagger(x) \frac{(-\hbar^2\partial_x^2)}{2m} a(x)$$

i.e. $$\boxed{\hat{H} = \hat{T} + \hat{V} = \int_0^L dx\ a^\dagger(x) \left[\frac{\hat{p}^2}{2m} + V(x)\right] a(x)}$$

where $\hat{p} = -i\hbar\partial_x$

▷ Two-body operators, i.e. operators which engage two-particles

E.g. symmetric pairwise interaction: $V(x,x') \equiv V(x',x)$ (such as Coulomb) acting between two-particle states

$$\hat{V} = \frac{1}{2}\int dx \int dx'\ |x,x'\rangle V(x,x') \langle x,x'|$$

When acting on many-particle states,

$$\hat{V}|x_1, x_2, \cdots x_N\rangle = \frac{1}{2}\sum_{n\neq m}^{N} V(x_n, x_m)|x_1, x_2, \cdots x_N\rangle$$

How can one express $\hat{V}$ in second quantised form?

might guess that

$$\hat{V} = \frac{1}{2}\int dx \int dx'\ a^\dagger(x)a^\dagger(x')V(x,x')a(x')a(x)$$

i.e. annihilation operators check for presence of particles at x and x' — if they exist, asign the potential energy and then recreate particles in correct order (viz. statistics). Factor of two for double-counting.

check:

$$\begin{aligned}
a^\dagger(x)a^\dagger(x')a(x')a(x)|x_1, x_2, \cdots x_N\rangle &= a^\dagger(x)a^\dagger(x')a(x')a(x) \quad a^\dagger(x_1)\cdots a^\dagger(x_N)|\Omega\rangle \\
&= \sum_{n=1}^{N} \zeta^{n-1}\delta(x-x_n)a^\dagger(x_n)\overbrace{a^\dagger(x')a(x')}^{n(x')} \quad a^\dagger(x_1)\cdots a^\dagger(x_{n-1})a^\dagger(x_{n+1})\cdots a^\dagger(x_N)|\Omega\rangle \\
&= \sum_{n=1}^{N} \zeta^{n-1}\delta(x-x_n) \sum_{m(\neq n)}^{N} \delta(x'-x_m)a^\dagger(x_n) \quad a^\dagger(x_1)\cdots a^\dagger(x_{n-1})a^\dagger(x_{n+1})\cdots a^\dagger(x_N)|\Omega\rangle \\
&= \sum_{n,m\neq n}^{N} \delta(x-x_n)\delta(x'-x_m)|x_1, x_2, \cdots x_N\rangle
\end{aligned}$$

then multiplying by $V(x,x')/2$, and integrate over x and $x' \;\mapsto \hat{V}$

N.B. $\frac{1}{2}\int dx \int dx'\; V(x,x')\hat{n}(x)\hat{n}(x')$ does *not* reproduce the two-body operator

▷ Turning to a non-diagonal basis

$$\boxed{\hat{\mathcal{O}}_2 = \sum_{\lambda\lambda'\mu\mu'} \mathcal{O}_{\mu,\mu',\lambda,\lambda'} a^\dagger_\mu a^\dagger_{\mu'} a_\lambda a_{\lambda'}, \qquad \mathcal{O}_{\mu,\mu',\lambda,\lambda'} \equiv \langle \mu,\mu'|\hat{\mathcal{O}}_2|\lambda,\lambda'\rangle}$$

▷ Applications of Second Quantisation

1. Phonons

   Oscillator states $|k\rangle$ form a Fock space:
   for each mode k, an arbitrary state of excitation can be created from the vacuum

   $$|k\rangle = a^\dagger_k|\Omega\rangle, \qquad a_k|\Omega\rangle = 0, \qquad [a_k, a^\dagger_{k'}] = \delta_{kk'}, \qquad \hat{H} = \sum_k \hbar\omega_k \left(a^\dagger_k a_k + 1/2\right)$$

   In this case, the Hamiltonian is diagonal: any state $|k_1, k_2, \cdots\rangle = a^\dagger_{k_1} a^\dagger_{k_2} \cdots |\Omega\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue $\hbar\omega_{k_1} + \hbar\omega_{k_2} + \cdots$

2. Interacting Electron Gas

   (i) Free-electron Hamiltonian

   $$\hat{H}^{(0)} = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\sigma} c_{k\sigma}, \qquad [c_{k\sigma}, c^\dagger_{k'\sigma'}] = \delta_{kk'}\delta_{\sigma\sigma'}$$

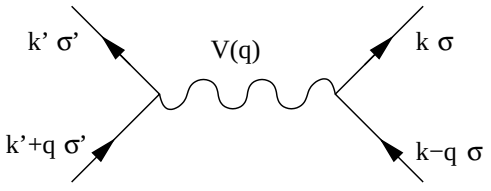
   also diagonal in plain wave basis

   (ii) Two-body interactions:

   $$\hat{H} = \hat{H}^{(0)} + \frac{1}{2}\int dx \int dx' \sum_{\sigma\sigma'} c^\dagger_\sigma(x) c^\dagger_{\sigma'}(x') V(x-x') c_{\sigma'}(x') c_\sigma(x)$$

   N.B. off-diagonal in Fourier basis! $\displaystyle\sum_{kk'q}\sum_{\sigma\sigma'} V(q)\, c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c_{k'+q,\sigma} c_{k-q,\sigma}$

   Feynman diagram:



▷ COMMENTS:

- Phonon Hamiltonian is example of 'free field theory':
  involves field operators at quadratic order but no higher...
- (whereas) electron Hamiltonian is typical of an interacting field theory:
  here there are two-body terms!
- As compared to free theories, analysis of interacting theories is infinitely harder...

▷ To familiarise ourselves with the second quantisation,
in the following lectures we will look at SEVERAL CASE STUDIES:

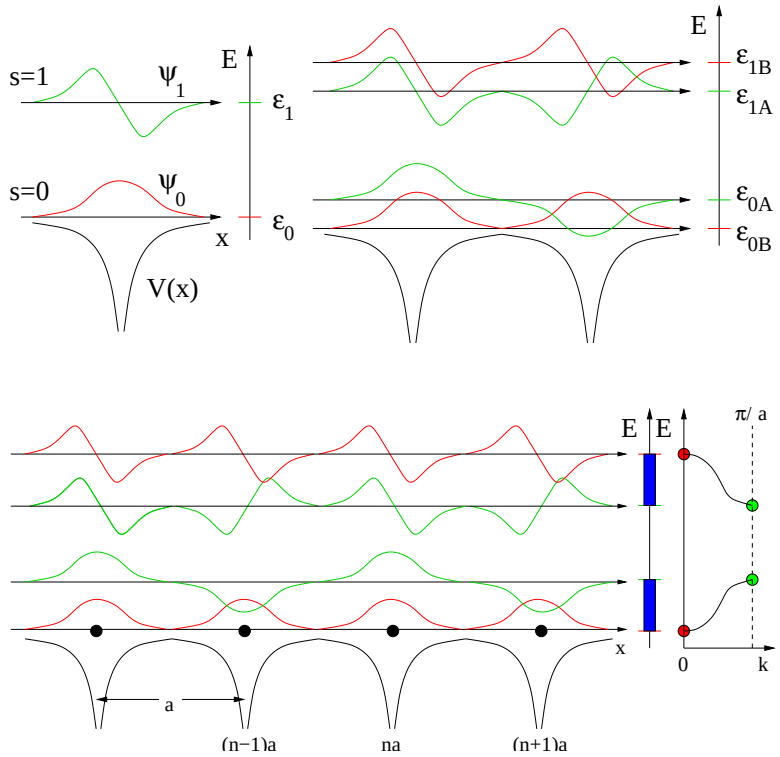
- 'Atomic limit' of strongly interacting electron gas:
  electron crystallisation and Mott transition
- Quantum magnetism
- Weakly interacting Bose gas

Lecture VI: Tight-binding and the Mott transition

According to band picture of non-interacting electrons, a 1/2-filled band of states is metallic. But strong Coulomb interaction of electrons can lead to a condensation or crystallisation of the electron gas into a solid, magnetic, insulating phase — Mott transition. Here we employ the second quantisation to explore the basis of this phenomenon.

▷ 'Atomic Limit' of crystal

How do atomic orbitals broaden into band states? `Transparencies`



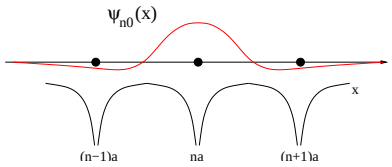
Weak overlap of tightly bound states ↦ narrow band:

Bloch states $|\psi_{ks}\rangle$, band index s, $k \in [-\pi/a, \pi/a]$

Bloch states can be used to define †'Wannier basis'

cf. discrete Fourier decomposition

$$|\psi_{ns}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{k\in[-\pi/a,\pi/a]}^{\text{B.Z.}} e^{-ikna}|\psi_{ks}\rangle, \qquad |\psi_{ks}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikna}|\psi_{ns}\rangle, \qquad k = \frac{2\pi}{Na}m$$



In 'atomic limit', Wannier states $|\psi_{ns}\rangle$ mirror atomic orbital $|s\rangle$ on site n

Field operators associated with Wannier basis: $\overbrace{|\psi_{ns}\rangle}^{c^\dagger_{ns\sigma}|\Omega\rangle} = \int dx \quad \overbrace{|x\rangle}^{c^\dagger_\sigma(x)|\Omega\rangle} \overbrace{\langle x|\psi_{ns}\rangle}^{\psi_{ns}(x)}$

$$c^\dagger_{ns\sigma} \equiv \int dx\ \psi_{ns}(x) c^\dagger_\sigma(x)$$

and using completeness (exercise) $\sum_{ns} \psi^*_{ns}(x')\psi_{ns}(x) = \delta(x-x')$

$$c^\dagger_\sigma(x) = \sum_{ns} \psi^*_{ns}(x) c^\dagger_{ns\sigma}, \qquad [c_{ns\sigma}, c^\dagger_{n's'\sigma'}]_+ = \delta_{\sigma\sigma'}\delta_{nn'}\delta_{ss'}$$

i.e. operators $c^\dagger_{ns\sigma}/c_{ns\sigma}$ create/annihilate electrons at site n in band s with spin σ

▷ In atomic limit, bands are well-separated in energy. If electron densities are low, one may project onto lowest band $s = 0$

Transforming to Wannier basis, interacting electron Hamiltonian takes form

$$\boxed{\hat{H} = \sum_{mn\sigma} t_{mn} c^\dagger_{m\sigma} c_{n\sigma} + \sum_{mnrs\sigma\sigma'} U_{mnrs} c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{r\sigma'} c_{s\sigma'}}$$

where "hopping" matrix elements: $t_{mn} = \langle \psi_m | \hat{H}^{(0)} | \psi_n \rangle = t^*_{nm}$ and "interaction parameters"

$$U_{mnrs} = \frac{1}{2} \int dx \int dx' \psi^*_m(x) \psi^*_n(x') \frac{e^2}{|x-x'|} \psi_r(x') \psi_s(x)$$

(For lowest band) representation is exact: but, in atomic limit, matrix elements decay exponentially with separation

(i) "Tight-binding" approximation:

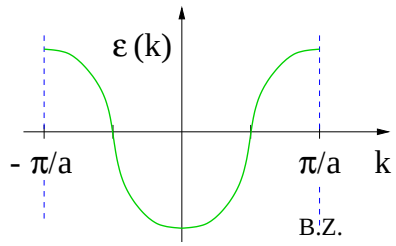
$$t_{mn} = \begin{cases} \epsilon & m = n \\ -t & mn \text{ neighbours} \\ 0 & \text{otherwise} \end{cases}, \qquad \hat{H}^{(0)} \simeq \sum_{n\sigma} \epsilon\ c^\dagger_{n\sigma} c_{n\sigma} - t \sum_{n\sigma} \left(c^\dagger_{n+1\sigma} c_{n\sigma} + \text{h.c.} \right)$$

In discrete Fourier basis: $c^\dagger_{n\sigma} = \frac{1}{\sqrt{N}} \sum_{k \in [-\pi/a, \pi/a]}^{\text{B.Z.}} e^{ikna} c^\dagger_{k\sigma}$

$$-t \sum_{n\sigma}^{N} \left(c^\dagger_{n+1\sigma} c_{n\sigma} + \text{h.c.} \right) = -t \sum_{kk'\sigma} \overbrace{\frac{1}{N} \sum_n e^{i(k-k')na}}^{\delta_{kk'}} e^{ika} c^\dagger_{k\sigma} c_{k'\sigma} + \text{h.c.} = -2t \sum_{k\sigma} \cos(ka)\ c^\dagger_{k\sigma} c_{k\sigma}$$

$$\boxed{\hat{H}^{(0)} = \sum_{k\sigma} (\epsilon - 2t \cos ka) c^\dagger_{k\sigma} c_{k\sigma}}$$

As expected, as $k \to 0$, spectrum becomes free electron-like: $\epsilon_k \to \epsilon - 2t + t(ka)^2 + \cdots$ (with $m^* = 1/2a^2t$)



(ii) Interaction

- Focusing on lattice sites $m \neq n$:
  1. Direct terms $U_{mnnm} \equiv V_{mn}$ — couple to density fluctuations: $\sum_{m\neq n} V_{mn}\hat{n}_m\hat{n}_n$
     $\rightsquigarrow$ potential for charge density wave instabilities
  2. Exchange coupling $J^F_{mn} \equiv U_{mnmn}$ (exercise — see lecture handout)

$$\sum_{m\neq n,\sigma\sigma'} U_{mnmn} c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{m\sigma'} c_{n\sigma} = -2 \sum_{m\neq n} J^F_{mn} \left(\hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n + \frac{1}{4}\hat{n}_m\hat{n}_n \right), \qquad \hat{\mathbf{S}}_m = \frac{1}{2} c^\dagger_{m\alpha} \sigma_{\alpha\beta} c_{m\beta}$$

  i.e. weak ferromagnetic coupling ($J_F > 0$) cf. Hund's rule in atoms
  spin alignment $\mapsto$ *symmetric spin state and asymmetric spatial state — lowers p.e.*

  But, in atomic limit, both t_{mn} and J^F_{mn} exponentially small in separation $|m-n|a$

- 'On-site' Coulomb or 'Hubbard' interaction

$$\sum_{n\sigma\sigma'} U_{nnnn} c^\dagger_{n\sigma} c^\dagger_{n\sigma'} c_{n\sigma'} c_{n\sigma} = U \sum_n \hat{n}_{n\uparrow}\hat{n}_{n\downarrow}, \qquad U \equiv 2U_{nnnn}$$

▷ Minimal model for strong interaction: Hubbard Hamiltonian

$$\boxed{\hat{H} = -t \sum_{n\sigma} (c^\dagger_{n+1\sigma} c_{n\sigma} + \text{h.c.}) + U \sum_n \hat{n}_{n\uparrow}\hat{n}_{n\downarrow}}$$

...could have been guessed on phenomenological grounds

`Transparencies on Mott-Insulators and the Magnetic State`

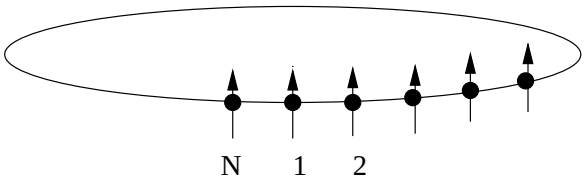
Lecture VII: Quantum Magnetism and the Ferromagnetic Chain

Following on from our investigation of the phonon and interacting electron system, we now turn to another example involving bosonic degrees of freedom — the problem of quantum magnetism.

▷ Spin S Quantum Heisenberg Magnet *spin analogue of discrete harmonic chain*

$$\boxed{\hat{H} = -J \sum_{m=1}^{N} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}}$$

periodic boundary conditions $\hat{\mathbf{S}}_{n+N} = \hat{\mathbf{S}}_n$



Sign of exchange coupling J depends on material parameters: Coulomb interaction tends to favour ferromagnetism $J > 0$ (cf. Hund's rule) while "superexchange" processes favour antiferromagnetism $J < 0$.

Aim: To uncover the ground states and nature of low-energy (collective) excitations

▷ Classical ground states?

- Ferromagnet: all spins aligned along a given (arbitrary) direction
  i.e. manifold of continuous degeneracy (cf. crystal)
- Antiferromagnet: (where possible) all neighbouring spins antiparallel — Néel state

▷ Quantum ground states:

$$\hat{H} = -J \sum_m \Big[\hat{S}^z_m \hat{S}^z_{m+1} + \overbrace{\hat{S}^x_m \hat{S}^x_{m+1} + \hat{S}^y_m \hat{S}^y_{m+1}}^{\frac{1}{2}(\hat{S}^+_m \hat{S}^-_{m+1} + \hat{S}^-_m \hat{S}^+_{m+1})} \Big]$$

where $\hat{S}^{\pm} = \hat{S}^x \pm i\hat{S}^y$ denotes spin raising/lowering operator

- Ferromagnet: as classical, e.g. $|\text{g.s.}\rangle = \otimes_{m=1}^{N} |S^z_m = S\rangle$
  No spin dynamics in $|\text{g.s.}\rangle$, i.e. no zero-point energy! (cf. phonons)
  Manifold of degeneracy explored by acting total spin lowering operator $\sum_m \hat{S}^-_m$
- Antiferromagnet: spin exchange interaction (viz. $\hat{S}^+_m \hat{S}^-_{m+1}$) $\rightsquigarrow$ zero point fluctuations which, depending on dimensionality, may or may not destroy ordered ground state

▷Elementary excitations?

Formation of magnetically ordered state breaks continuous spin rotation symmetry ⇝ low-energy collective excitations (spin waves or magnons) — cf. phonons in a crystal

Example of general principle known as Goldstone's theorem

However, as with lattice vibrations, 'general theory' is nonlinear
fortunately, low-energy excitations described by free theory

To see this, for large spin S, it is helpful to switch to a spin representation in which deviations from $|\text{g.s.}\rangle$ are parameterised as bosons:

$$\begin{array}{ll} |S^z = S\rangle & |n = 0\rangle \\ |S^z = S-1\rangle & |n = 1\rangle \\ |S^z = S-2\rangle & |n = 2\rangle \\ \vdots & \vdots \\ |S^z = -S\rangle & |n = 2S\rangle \end{array}$$

i.e. a maximum of n bosons per lattice site ("softcore" constraint)

For ferromagnetic ground state with spins oriented along z-axis,
the ground state coincides with the vacuum state $|\text{g.s.}\rangle \equiv |\Omega\rangle$, i.e. $a_m|\Omega\rangle = 0$

Mapping useful when elementary spin wave excitation involves $n \ll 2S$

▷ Mapping of operators: $\hat{S}^z$, $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$?
with $\hbar = 1$, operators obey quantum spin algebra

$$[\hat{S}^\alpha, \hat{S}^\beta] = i\epsilon^{\alpha\beta\gamma}\hat{S}^\gamma \qquad \rightsquigarrow \qquad [\hat{S}^+, \hat{S}^-] = 2\hat{S}^z, \qquad [\hat{S}^z, \hat{S}^\pm] = \pm\hat{S}^\pm$$

cf. bosons: $[a, a^\dagger] = 1, \qquad n = a^\dagger a$

According to mapping, $\hat{S}^z = S - a^\dagger a$;
therefore, to leading order in $S \gg 1$ (spin-wave approximation),

$$\hat{S}^- \simeq (2S)^{1/2} a^\dagger, \qquad \hat{S}^+ \simeq (2S)^{1/2} a$$

In fact, exact equivalence provided by Holstein-Primakoff transformation

$$\hat{S}^- = a^\dagger \left(2S - a^\dagger a\right)^{1/2}, \qquad \hat{S}^+ = (\hat{S}^-)^\dagger, \qquad \hat{S}^z = S - a^\dagger a$$

▷ Applied to FERROMAGNETIC HEISENBERG SPIN S CHAIN, 'spin-wave' approximation:

$$\begin{aligned} \hat{H} &= -J\sum_{m=1}^{N}\left\{\hat{S}^z_m\hat{S}^z_{m+1} + \frac{1}{2}(\hat{S}^+_m\hat{S}^-_{m+1} + \hat{S}^-_m\hat{S}^+_{m+1})\right\} \\ &= -J\sum_m\left\{S^2 - S(a^\dagger_m a_m - a^\dagger_{m+1}a_{m+1}) + S(a_m a^\dagger_{m+1} + a^\dagger_m a_{m+1}) + O(S^0)\right\} \\ &= -J\sum_m\left\{S^2 - 2Sa^\dagger_m a_m + S\left(a^\dagger_m a_{m+1} + \text{h.c.}\right) + O(S^0)\right\} \end{aligned}$$

with p.b.c. $\hat{S}_{m+N} = \hat{S}_m$ and $a_{m+N} = a_m$

To leading order in S, Hamiltionian is bilinear in Bose operators;
diagonalised by discrete Fourier transform (exercise)

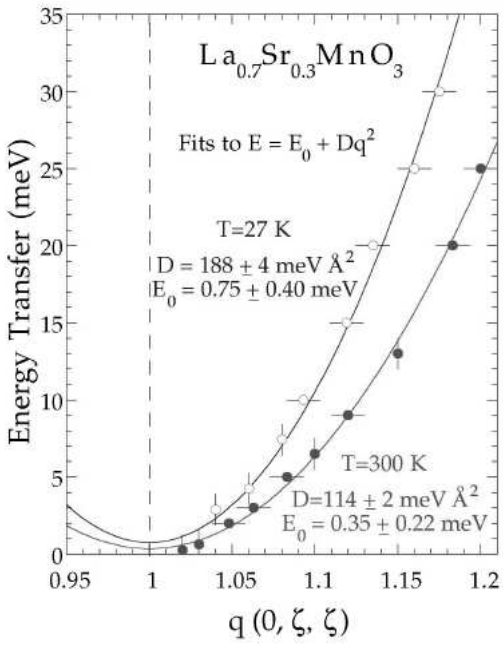
$$a_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikn} a_n, \qquad a_n = \frac{1}{\sqrt{N}} \sum_{k}^{\text{B.Z.}} e^{-ikn} a_k, \qquad [a_k, a_{k'}^\dagger] = \delta_{kk'}$$

noting $\sum_n e^{i(k-k')n} = N\delta_{kk'}$

$$\hat{H} = -JNS^2 + \sum_{k}^{\text{B.Z.}} \omega_k a_k^\dagger a_k + O(S^0), \qquad \omega_k = 2JS(1-\cos k) = 4JS\sin^2(k/2)$$

cf. free-particle spectrum

Terms of higher order in $S \rightsquigarrow$ spin-wave interactions

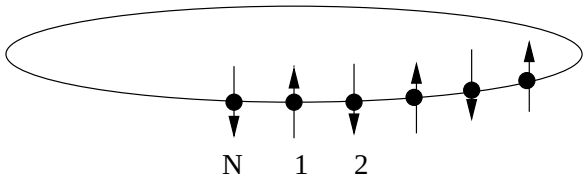


Lecture VIII: Quantum Antiferromagnetism

We have seen that the quantum Heisenberg Ferromagnetic spin chain is characterised by a magnetically ordered ground state with free particle-like elementary spin wave excitations — magnons. What happens in the antiferromagnetic system?

▷ Antiferromagnet Heisenberg spin S chain

$$\hat{H} = J\sum_{m=1}^{N} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}, \qquad J>0, \qquad \text{p.b.c. } \hat{\mathbf{S}}_{m+N} = \hat{\mathbf{S}}_m$$



Classical ground state (Néel) no longer an eigenstate
— nevertheless, it serves as reference for spin-wave expansion

In this case, it is convenient to implement transformation in which spins on one sublattice, say B, are rotated through 180^o about the x-axis,

$$\text{i.e.} \qquad \hat{S}^x_B \longmapsto \hat{S}^x_B, \qquad \hat{S}^y_B \longmapsto -\hat{S}^y_B, \qquad \hat{S}^z_B \longmapsto -\hat{S}^z_B$$

Note that transformation is said to be canonical:
i.e. it respects the canonical commutation relations

$$\hat{H} = -J\sum_m \left[\hat{S}^z_m\hat{S}^z_{m+1} - \frac{1}{2}(\hat{S}^+_m\hat{S}^+_{m+1} + \hat{S}^-_m\hat{S}^-_{m+1})\right]$$

In rotated frame, classical ground state is ferromagnetic
but $\hat{S}^-_m\hat{S}^-_{m+1} \rightsquigarrow$ zero-point fluctuations (ZPF)

Applying spin wave approximation: $\hat{S}^z_m = S - a^\dagger_m a_m$, $\hat{S}^-_m \simeq (2S)^{1/2}a^\dagger_m$, etc.

$$\hat{H} = -NJS^2 + JS\sum_m \left[2a^\dagger_m a_m + a_m a_{m+1} + a^\dagger_m a^\dagger_{m+1}\right] + O(S^0)$$

$\rightsquigarrow$ processes that do not conserve particle number! (ZPF)

Turning to Fourier representation: $a_m = \frac{1}{N^{1/2}}\sum_k e^{-ikm}a_k$, etc., and using

$$\sum_{m=1}^{N} a_m a_{m+1} = \sum_{kk'} \overbrace{\frac{1}{N}\sum_{m=1}^{N} e^{-i(k+k')m}}^{\delta_{k+k',0}} e^{-ik} = \sum_k a_k a_{-k} e^{-ik} \equiv \sum_k a_k a_{-k} \overbrace{\frac{1}{2}(e^{ik}+e^{-ik})}^{\gamma_k = \cos k}$$

$$\hat{H} = -NJS(S+1) + JS\sum_k \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} + O(S^0)$$

To diagonalise $\hat{H}$, might think of making unitary transformation. However, transformation must preserve canonical commutation relations. Achieved by (exercis, PS II)

▷ BOGOLIUBOV TRANSFORMATION: (cf. Lorentz boost — preserves metric $g = \sigma_z$)

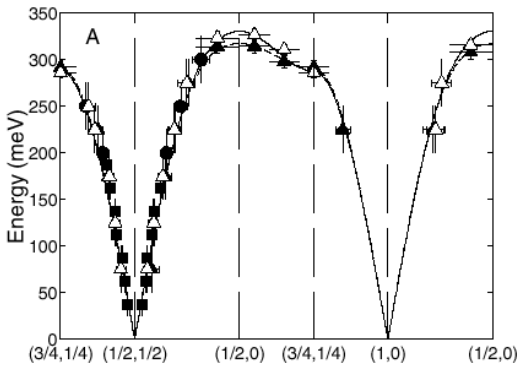
$$\begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix}$$

Off-diagonal terms removed by setting $\tanh(2\theta_k) = \gamma_k$

$$\begin{aligned} \hat{H} &= -NJS(S+1) + JS\sum_k |\sin k| \left(\alpha_k^\dagger\alpha_k + \alpha_{-k}\alpha_{-k}^\dagger\right) + O(S^0) \\ &= -NJS(S+1) + 2JS\sum_k |\sin k| \left[\alpha_k^\dagger\alpha_k + \frac{1}{2}\right] + O(S^0) \end{aligned}$$

$\rightsquigarrow$ linear (cf. relativistic) excitation spectrum (cf. phonons, photons, etc.)

Experiment?



▷ Average Magnetisation

- Do thermal fluctuations destroy magnetic order in ferromagnet?

$$\langle M\rangle = \langle \text{g.s.}|\frac{1}{N}\sum_i \hat{S}_i^z|\text{g.s.}\rangle = S - \langle \text{g.s.}|\frac{1}{N}\sum_i a_i^\dagger a_i|\text{g.s.}\rangle = S - \langle \text{g.s.}|\frac{1}{N}\sum_k a_k^\dagger a_k|\text{g.s.}\rangle$$

$$= S - \int \frac{d^dk}{(2\pi)^d} \overbrace{\frac{1}{e^{\omega_k/k_\mathrm{B}T}-1}}^{n_\mathrm{B}(T)} \overset{k_\mathrm{B}T\gg JS}{\sim} S - \frac{k_\mathrm{B}T}{JS}\int_0^{1/a} k^{d-1}dk\frac{1}{k^2}$$

divergent for $T \neq 0$ in $d \leq 2$

i.e. In $d \leq 2$ long-range order destroyed by thermal fluctuations at any non-zero temperature (example of general principle: Mermin-Wagner theorem)

- At $T = 0$, do ZPF destroy long-range order in antiferromagnet?

  Referring to sublattice magnetisation (cf. $\langle m \rangle$ in rotated frame)

$$\langle M_{\text{s.l.}} \rangle = \langle \text{g.s.} | \frac{1}{N} \sum_i \hat{S}_i^z | \text{g.s.} \rangle = S - \langle \text{g.s.} | \frac{1}{N} \sum_k a_k^\dagger a_k | \text{g.s.} \rangle = S - \frac{1}{N} \sum_k \sinh^2 \theta_k$$

$$= S - \int \frac{d^d k}{(2\pi)^d} \frac{1}{2} \left[(1 - \gamma_k^2)^{-1/2} - 1 \right] \sim \int_0^{1/a} k^{d-1} dk \frac{1}{k}$$

  diverges in $d = 1$!

  i.e. quantum fluctuations destroy antiferromagnetic order in $d = 1$ even at $T = 0$!
  spin liquid phase

▷ FRUSTRATION

AF exchange interaction on "bipartite" lattice $\rightsquigarrow$ Néel ordering
which, in $d > 1$, survives quantum ZPF

For non-bipartite lattice (such as triangular),
AF exchange interaction is said to be frustrated...

Can ZPF lead to spin liquid in higher dimensions...? subject of current research!

Lecture IX: Bogoliubov Theory of weakly interacting Bose gas

Although strong interaction effects can lead to the formation of novel ground states of the electron system, the properties of the weakly interacting system mirror closely the trivial behaviour of the non-interacting fermi gas. By contrast, even in the weakly interacting system, the Bose gas has the capacity to form a Bose-Einstein condensed phase. The aim of this lecture is to explore the nature of the ground state and the character of the elementary excitation spectrum in the condensed phase.

▷ Weakly interacting Bose gas

Consider a system of N bosons confined to a volume L^d

In the non-interacting system, at $T = 0$, all bosons are condensed in the lowest energy single-particle state, viz. $|\text{g.s.}\rangle = \frac{1}{N!}(a_0^\dagger)^N|\Omega\rangle$

Aim: How is ground state and spectrum of elementary excitations influenced by weak interaction?

$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \overbrace{\frac{1}{2}\int d^dx \int d^dx'\, a^\dagger(\mathbf{x})a^\dagger(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')a(\mathbf{x}')a(\mathbf{x})}^{\hat{H}_I}$$

$V(\mathbf{x}-\mathbf{x}')$ — pairwise particle interaction

In Fourier basis, with $a(\mathbf{x}) = \frac{1}{L^{d/2}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}$ and $V(\mathbf{q}) = \int d^dx\, e^{-i\mathbf{q}\cdot\mathbf{x}} V(\mathbf{x})$

$$\hat{H}_I = \frac{1}{2L^d}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V(\mathbf{q})\, a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} a_{\mathbf{k}'+\mathbf{q}}$$

If interaction is weak, in condensed phase, one may assume that the lowest-lying single-particle state is still macroscopically occupied, i.e. $N_0/N = \mathcal{O}(1)$

Therefore, since $\hat{N}_0 = a_{k=0}^\dagger a_{k=0} = \mathcal{O}(N) \gg 1$ and $a_0 a_0^\dagger - a_0^\dagger a_0 = 1$, to a good approximation, a_0 and $a_0^\dagger$ can be replaced by the ordinary c-number $\sqrt{N_0}$

Taking (for simplicity) $V(\mathbf{q}) = V$ const., i.e. a contact interaction, expansion in N_0 obtains

$$\hat{H}_I = \frac{V}{2L^d}N_0^2 + \frac{V}{L^d}N_0\sum_{\mathbf{k}\neq 0}\left[a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}} + \frac{1}{2}\left(a_{-\mathbf{k}}a_{\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger\right)\right] + O(N_0^0)$$

cf. quantum AF in spin-wave approximation

▷ Physical interpretation of components:

- $Va_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ represents the 'Hartree-Fock energy' of excited particles interacting with condensate — *Note that the contact nature of the interaction disguises the presence of the direct and exchange contributions*

- $V(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}})$ represents creation or annihilation of excited particles from the condensate; *Note that, in this approximation, total no. of particles is not conserved*

Finally, using the identity $N = N_0 + \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}}a_{\mathbf{k}}$ to trade N_0 for N,

$$\hat{H} = \frac{VnN}{2} + \sum_{\mathbf{k}\neq 0}\left[\left(\epsilon^0_{\mathbf{k}} + Vn\right)\, a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + \frac{Vn}{2}\left(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}}\right)\right]$$

where $n = N/L^d$ denotes number density and $\epsilon^0_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2m}$

As with quantum AF, $\hat{H}$ diagonalised by Bogoluibov transformation:

$$\begin{pmatrix} a_{\mathbf{k}} \\ a^\dagger_{-\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \cosh\theta_{\mathbf{k}} & -\sinh\theta_k \\ -\sinh\theta_{\mathbf{k}} & \cosh\theta_{\mathbf{k}} \end{pmatrix}\begin{pmatrix} \alpha_{\mathbf{k}} \\ \alpha^\dagger_{-\mathbf{k}} \end{pmatrix}$$

Left as exercise to show that, when $\tanh(2\theta_k) = Vn/(\epsilon^0_{\mathbf{k}} + Vn)$,

$$\hat{H} = \frac{VnN}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon^0_{\mathbf{k}} + nV) + \sum_{\mathbf{k}\neq 0}\overbrace{\left[\left(\epsilon^0_{\mathbf{k}} + Vn\right)^2 - (Vn)^2\right]^{1/2}}^{\epsilon_{\mathbf{k}}}\left(\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}} + \frac{1}{2}\right)$$

In particular, for $|\mathbf{k}| \to 0$, spectrum of low-energy excitations scales as $\epsilon(\mathbf{k}) \simeq \hbar c|\mathbf{k}|$ with $c = (Vn/m)^{1/2}$

At high energies ($k > k_0 = mc/\hbar$), spectrum becomes free particle-like

▷ †Ground state wavefunction: defined by condition $\alpha_{\mathbf{k}}|\text{g.s.}\rangle$

Since Bogoluibov transformation can be written as $\alpha_{\mathbf{k}} = Ua_{\mathbf{k}}U^{-1}$ where (exercise)

$$U = \exp\left[\sum_{\mathbf{k}\neq 0}\frac{\theta_{\mathbf{k}}}{2}(a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}} - a_{\mathbf{k}}a_{-\mathbf{k}})\right]$$

may infer g.s. $|\Phi_V\rangle$ from non-interacting g.s. $|\Phi_0\rangle$ as $|\Phi_V\rangle = U|\Phi_0\rangle$

Proof: since, for $V = 0$, all particles are in the $\mathbf{k} = 0$ state,

$$0 = a_{\mathbf{k}\neq 0}|\Phi_0\rangle = U^{-1}\overbrace{Ua_{\mathbf{k}}U^{-1}}^{\alpha_{\mathbf{k}}}U|\Phi_0\rangle$$

▷ †Depletion of condensate due to interaction

$$\frac{N - N_0}{N} = \frac{1}{N}\sum_{\mathbf{k}\neq 0}\langle\text{g.s.}|a^\dagger_{\mathbf{k}}a_{\mathbf{k}}|\text{g.s.}\rangle = \frac{1}{N}\sum_{\mathbf{k}\neq 0}\sinh^2\theta_{\mathbf{k}} = \frac{1}{n}\int\frac{d^dk}{(2\pi)^3}\sinh^2\theta_{\mathbf{k}} \overset{\text{exercise}}{=} \frac{1}{3\pi^2 n}k_0^3$$

i.e. ca. one particle per 'coherence length' $\xi \sim 1/k_0$

Recast using scattering length (cf. TP2) of contact interaction $V = 4\pi\hbar^2 a/m$,

$$\frac{N - N_0}{N} = \frac{8}{3\sqrt{\pi}}(na^3)^{1/2}$$

▷ †Ground state energy

$$E_0 = \frac{VnN}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon^0_{\mathbf{k}} + nV - \epsilon_{\mathbf{k}} - \frac{(nV)^2}{2\epsilon^0_{\mathbf{k}}})$$

(where extra term controls unphysical UV divergence
required by contact nature of potential)

$$\frac{E_0}{L^d} = \frac{n^2 V}{2}\left[1 + \frac{128}{15\sqrt{\pi}}(na^3)^{1/2}\right]$$

▷ Experiment? `transparencies`

When cooled to $T \sim 2K$, liquid ^{4}He undergoes
transition to Bose-Einstein condensed state

Neutron scattering measurements can be used to infer spectrum of
collective excitations

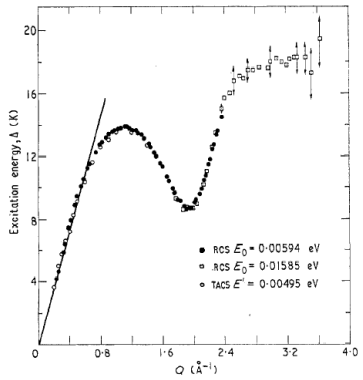


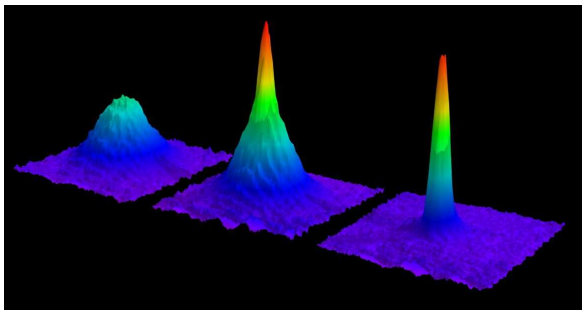
Figure 9. The dispersion curve for He II for the elementary excitations at $T = 1{\cdot}1$ K and $P \simeq 0$. Data obtained by rotating crystal spectrometer (RCS) and triple axis crystal spectrometer (TACS) as indicated. From Cowley and Woods (1971).

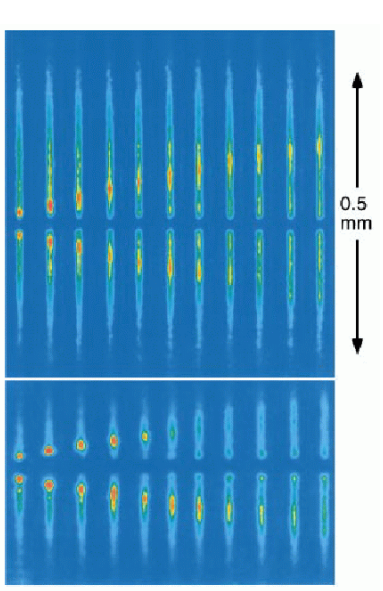
In Helium, steric interactions are strong and at higher energy scales
an important second branch of excitations known as rotons appear

A second example of BEC is presented by ultracold atomic gases:

By confining atoms to a magnetic trap, time of flight measurements
can be used to monitor momentum distribution of condensate

Moreover, the perturbation imposed by a laser due to the optical
dipole interaction provides a means to measure the sound wave velocity





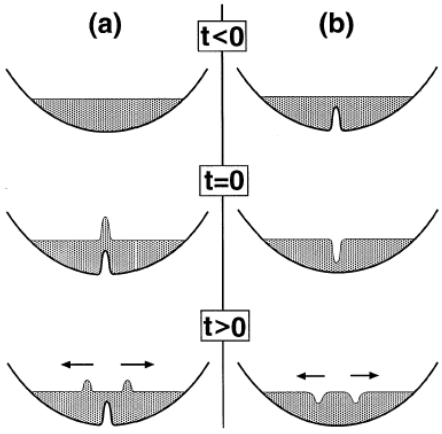


FIG. 1. Excitations of wave packets in a Bose-Einstein condensate. A condensate is confined in the potential of a magnetic trap. At time $t = 0$, a focused, blue-detuned laser beam is suddenly switched on (a) or off (b) and, by the optical dipole force, creates, respectively, two positive or negative pertubations in density which propagate at the speed of sound.

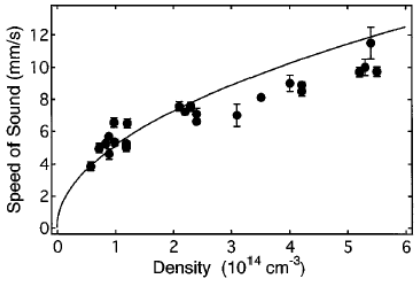


FIG. 4. Speed of sound versus condensate peak density. The solid line is the speed of sound [Eq. (2)] using the maximum cloud density [Eq. (4)] with no adjustable parameter. The error bars show only the statistical error.

Lecture X: Feynman Path Integral

Although the second quantisation provides a convenient formulation of many-body systems, it admits solution only for systems that are effectively free. In our choice of applications, we were careful to consider only those systems for which interaction effects could be considered as small, e.g. large spin in quantum magnetism of weak interaction in the dilute Bose gas. Yet interactions can have a profound effect leading to transitions to new phases with elementary excitations very different from the bare particles. To address such phenomena, it is necessary to switch to a new formulation of quantum mechanics. However, to do so, it will be necessary to leave behind many-body theories and return to single-particle systems.

▷ Motivation:

- Alternative formulation of QM (cf. canonical quantisation)
- Close to classical construction — i.e. semi-classics easily retrieved
- Effective formulation of non-perturbative approaches
- Prototype of higher-dimensional field theories

▷ Time-dependent Schrödinger equation

$$\boxed{i\hbar\partial_t|\Psi\rangle = \hat{H}|\Psi\rangle}$$

Formal solution: $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = \sum_n e^{-iE_nt/\hbar}|n\rangle\langle n|\psi(0)\rangle$

▷ Time-evolution operator

$$|\Psi(t')\rangle = \hat{U}(t',t)|\Psi(t)\rangle, \qquad \hat{U}(t',t) = e^{-\frac{i}{\hbar}\hat{H}(t'-t)}\theta(t'-t) \qquad \text{N.B. Causal}$$

- Real-space representation:

$$\Psi(q',t') \equiv \langle q'|\Psi(t')\rangle = \langle q'|\hat{U}(t',t)\int dq|q\rangle\langle q| \quad \wedge \quad |\Psi(t)\rangle = \int dq\, U(q',t';q,t)\Psi(q,t),$$

where $U(q',t';q,t) = \langle q'|e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|q\rangle\theta(t'-t)$ — propagator or Green function

$$\left(i\hbar\partial_{t'} - \hat{H}\right)\hat{U}(t'-t) = i\hbar\delta(t'-t) \qquad \text{N.B. } \partial_{t'}\theta(t'-t) = \delta(t'-t)$$

Physically: $U(q',t';q,t)$ describes probability amplitude for particle to propagate from q at time t to q' at time t'

▷ Construction of Path Integral

Feynman's idea: separate time evolution into $N \to \infty$ discrete time steps $\Delta t = t/N$

$$e^{-i\hat{H}t/\hbar} = [e^{-i\hat{H}\Delta t/\hbar}]^N$$

Then separate the operator content so that momentum operators stand to the left and position operators to the right:

$$e^{-i\hat{H}\Delta t/\hbar} = e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar} + O(\Delta t^2)$$

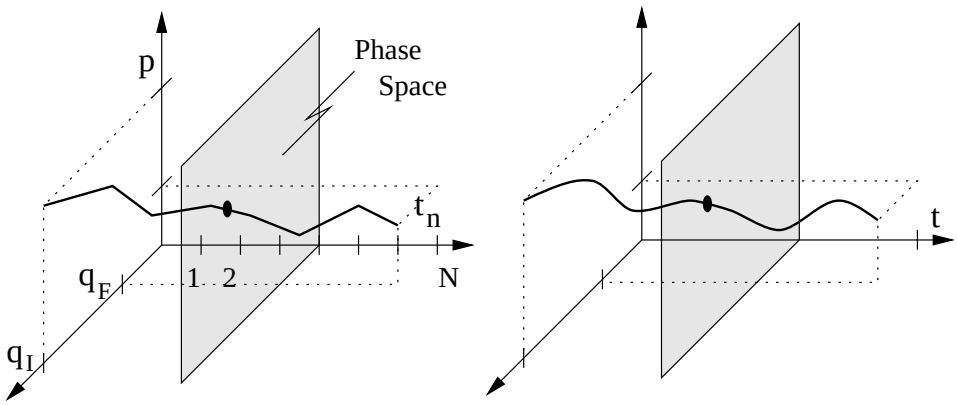
$$\langle q_F|[e^{-i\hat{H}\Delta t/\hbar}]^N|q_I\rangle \simeq \langle q_F|_\wedge e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar}{}_\wedge \cdots {}_\wedge e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar}|q_I\rangle$$

Inserting at $\wedge$ resol. of id. $= \int_{-\infty}^{\infty} dq_n \int_{-\infty}^{\infty} dp_n |q_n\rangle\langle q_n|p_n\rangle\langle p_n|$, and using $\langle q|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{iqp/\hbar}$,

$$e^{-i\hat{V}\Delta t/\hbar}|q_n\rangle\langle q_n|p_n\rangle\langle p_n|e^{-i\hat{T}\Delta t/\hbar} = |q_n\rangle e^{-iV(q_n)\Delta t/\hbar}\langle q_n|p_n\rangle e^{-iT(p_n)\Delta t/\hbar}\langle p_n|,$$

$$\text{and} \quad \langle p_{n+1}|q_n\rangle\langle q_n|p_n\rangle = \frac{1}{2\pi\hbar}e^{iq_n(p_n-p_{n+1})/\hbar}$$

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{\substack{q_N=q_F,q_0=q_I}} \prod_{n=1}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \exp\left[-\frac{i}{\hbar}\Delta t \sum_{n=0}^{N-1}\left(V(q_n) + T(p_{n+1}) - p_{n+1}\frac{q_{n+1}-q_n}{\Delta t}\right)\right]$$



i.e. at each time step, integration over the classical phase space coords. (q_n, p_n)

Contributions from trajectories where $(q_{n+1} - q_n)p_{n+1} > \hbar$ are negligible
— motivates continuum limit

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \overbrace{\int_{q(t)=q_F,q(0)=q_I} D(q,p)}^{\int_0^t dt'} \Big/ \int_{\substack{q_N=q_F,q_0=q_I}} \prod_{n=1}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \exp\Big[-\frac{i}{\hbar}\overbrace{\Delta t \sum_{n=0}^{N-1}}^{\int_0^t dt'} \big(\overbrace{V(q_n) + T(p_{n+1})}^{H(q,p|_{t'=t_n})} - \overbrace{p_{n+1}\frac{q_{n+1}-q_n}{\Delta t}}^{p\dot{q}|_{t'=t_n}}\big)\Big]$$

▷ Hamiltonian formulation of Feynman Path Integral:

Propagator expressed as FUNCTIONAL INTEGRAL

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{q(t)=q_F,q(0)=q_I} D(q,p) \exp\Big[\frac{i}{\hbar}\overbrace{\int_0^t dt' \overbrace{(p\dot{q} - H(p,q))}^{\text{Lagrangian}}}^{\text{Action}}\Big]$$

Quantum transition amplitude expressed as sum over all possible phase space trajectories (subject to appropriate b.c.) and weighted by classical action

▷ Lagrangian formulation: for "free-particle" Hamiltonian $H(p,q) = p^2/2m + V(q)$

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{q(t)=q_F, q(0)=q_I} Dq\; e^{-(i/\hbar)\int_0^t dt' V(q)} \int Dp \overbrace{\exp\left[-\frac{i}{\hbar}\int_0^t dt' \left(\frac{p^2}{2m} - p\dot{q}\right)\right]}^{\text{Gaussian integral on p}}$$

$$\frac{p^2}{2m} - p\dot{q} \mapsto \frac{1}{2m}\overbrace{(p - m\dot{q})^2}^{p'^2} - \frac{1}{2}m\dot{q}^2$$

Functional integral justified by discretisation

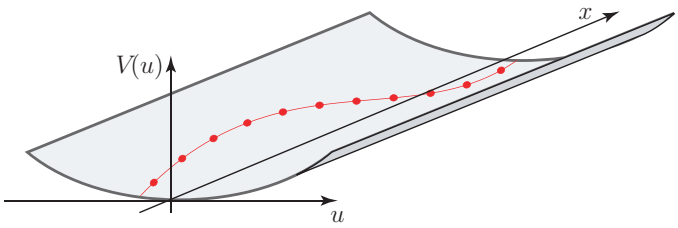
$$\boxed{\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{q(t)=q_F, q(0)=q_I} Dq \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(\frac{m\dot{q}^2}{2} - V(q)\right)\right]}$$

$$Dq \equiv \lim_{N\to\infty}\left(\frac{Nm}{it2\pi\hbar}\right)^{N/2}\prod_{n=1}^{N-1} dq_n$$

Lecture XI: Statistical Mechanics and Semi-Classics

▷ Connection of Path Integral to Classical Statistical Mechanics

Consider flexible string held under constant tension and confined to 'gutter' potential



Potential energy stored in spring due to line tension:

$$\text{from segment } x \text{ to } x+dx,\ dV_T = T\,\overbrace{[(dx^2+du^2)^{1/2}-dx]}^{\text{extension}} \simeq T\,dx\,(\partial_x u)^2/2$$

$$V_T[\partial_x u] \equiv \int dV_T = \frac{1}{2}\int_0^L dx\ T\,(\partial_x u(x))^2$$

External (gutter) potential: $V_{\rm ext}[u] \equiv \int_0^L dx\ V[u(x)]$

According to Boltzmann principle, equilibrium partition function

$$\boxed{\mathcal{Z} = \mathrm{tr}\left(e^{-\beta F}\right) = \int Du(x)\ \exp\left[-\beta\int_0^L dx\left(\frac{T}{2}(\partial_x u)^2 + V(u)\right)\right]}$$

cf. quantum mechanical transmission amplitude

▷ Mapping:

$$\mathcal{Z} = \int_{\rm b.c.} Dq(t)\ \exp\left[\frac{i}{\hbar}\int_0^t dt'\left(\frac{m\dot{q}^2}{2} - V(q)\right)\right]$$

Wick rotation $t \to -i\tau \mapsto$ imaginary (Euclidean) time path integral

$$\int_0^t i dt'\ (\partial_{t'} q)^2 \longrightarrow -\int_0^\tau d\tau'(\partial_{\tau'} q)^2, \qquad -\int_0^t i dt' V(q) \longrightarrow -\int_0^\tau d\tau' V(q)$$

$$\mathcal{Z} = \int_{\rm b.c.} Dq \exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau'\left(\frac{m}{2}(\partial_{\tau'} q)^2 + V(q)\right)\right] \qquad \text{N.B. change of relative sign!}$$

(a) Classical partition function of one-dimensional system
coincides with quantum mechanical amplitude

$$\mathcal{Z} = \int dq\ \langle q|e^{-i\hat{H}t/\hbar}|q\rangle\Big|_{t=-i\tau}$$

where time is imaginary, and $\hbar$ plays the role of temperature

More generally, path integral for d-dimensional quantum system
corresponds to classical statistical mechanics of $d+1$-dimensional system

(b) Quantum partition function

$$\mathcal{Z} = \mathrm{tr}(e^{-\beta\hat{H}}) = \int dq\, \langle q|e^{-\beta\hat{H}}|q\rangle$$

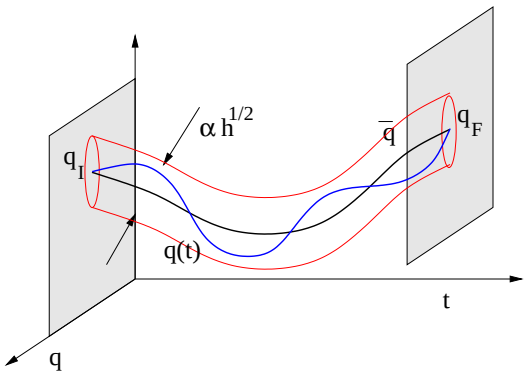
i.e. $\mathcal{Z}$ can be interpreted through dynamical transition amplitude $\langle q|e^{-i\hat{H}t/\hbar}|q\rangle$
evaluated at imaginary time $t = -i\hbar\beta$.

(c) In semi-classical limit ($\hbar \to 0$), PI dominated by stationary configurations of action
$S[p,q] = \int dt(p\dot{q} - H(p,q))$

$$\begin{aligned}
\delta S &= S[p+\delta p, q+\delta q] - S[p,q] \\
&= \int dt\, [\delta p\dot{q} + p\delta\dot{q} - \delta p\partial_p H - \delta q\partial_q H] + O(\delta p^2, \delta q^2, \delta p\delta q) \\
&= \int dt\, [\delta p\,(\dot{q} - \partial_p H) + \delta q\,(-\dot{p} - \partial_q H)] + O(\delta p^2, \delta q^2, \delta p\delta q)
\end{aligned}$$

i.e. Hamilton's classical e.o.m.: $\dot{q} = \partial_p H$, $\dot{p} = -\partial_q H$ with b.c. $q(0) = q_I$, $q(t) = q_F$

(Similarly, with Lagrangian formulation : $\delta S = 0 \Rightarrow (d_t\partial_{\dot{q}} - \partial_q)\, L(q,\dot{q}) = 0$)



Contributions to PI from fluctuations around classical paths?

Usually, exact evaluation of PI impossible — resort to approximation schemes...

▷ Saddle-point and Stationary Phase analysis

Consider integral over single variable

$$I = \int_{-\infty}^{\infty} dz\, e^{-f(z)}$$

Integral dominated by minima of $f(z)$; suppose unique i.e. $f'(z_0) = 0$

Taylor expand around minimum: $f(z) = f(z_0) + (z - z_0)\overbrace{f'(z_0)}^{\mapsto 0} + \frac{1}{2}(z - z_0)^2 f''(z_0) + \cdots$

$$I \simeq e^{-f(z_0)} \int_{-\infty}^{\infty} dz\, e^{-(z-z_0)^2 f''(z_0)/2} = \sqrt{\frac{2\pi}{f''(z_0)}} e^{-f(z_0)}$$

Example : $\Gamma(s+1) = \int_0^\infty dz z^s e^{-z} = \int_0^\infty dz\, e^{-f(z)}, \qquad f(z) = z - s\ln z$

$f'(z) = 1 - s/z$ i.e. $z_0 = s$, $f''(z_0) = s/z_0^2 = 1/s$
i.e. $\Gamma(s+1) \simeq \sqrt{2\pi s} e^{-(s - s\ln s)}$ — Stirling's formula

If minima not on contour of integration — deform contour through saddle-point
e.g. $\Gamma(s+1)$, s complex

What if exponent complex? Fast phase fluctuations $\rightsquigarrow$ cancellation
i.e. expand around region of slowest (i.e. stationary) phase and use identity

$$\int_{-\infty}^{\infty} dz\, e^{iaz^2/2} = \sqrt{\frac{2\pi}{a}} e^{i\pi/4}$$

▷ Can we apply same approach to analyse the FPI?

Yes: but we we must develop new technology;
basic tool of QFT — the Gaussian functional integral!

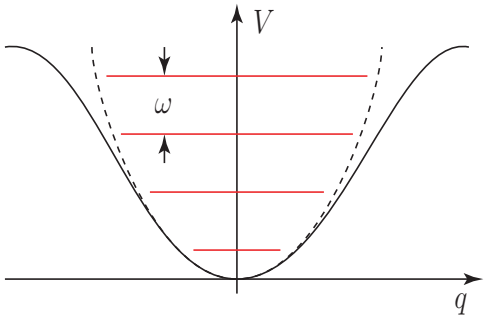
Lecture XII: Applications of the Feynman Path Integral

▷ Digression: Free particle propagator (exercise) cf. diffusion

$$G_{\rm free}(q_F,q_I;t)\equiv\langle q_F|e^{-i\hat{p}^2t/2m\hbar}|q_I\rangle\Theta(t)=\left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\exp\left[\frac{i}{\hbar}\frac{m(q_F-q_I)^2}{2t}\right]\Theta(t)$$

Difficult to derive from PI(!), but useful for normalization

▷ Quantum Particle in a Single (Symmetric) Well: $V(q)=V(-q)$



e.g. QM amplitude

$$G(0,0;t)\equiv\langle 0|e^{-i\hat{H}t/\hbar}|0\rangle\,\Theta(t)=\int_{q(t)=q(0)=0}Dq\exp\left[\frac{i}{\hbar}\int_0^t dt'\left(\frac{m\dot{q}^2}{2}-V(q)\right)\right]$$

▷ Evaluate PI by stationary phase approximation: *general recipe*

(i) Parameterise path as $q(t)=q_{\rm cl}(t)+r(t)$ and expand action in $r(t)$

$$S[\bar{q}+r]=\int_0^t dt'\Big[\frac{m}{2}\overbrace{\dot{q}_{\rm cl}{}^2+2\dot{q}_{\rm cl}\dot{r}+\dot{r}^2}^{(\dot{q}_{\rm cl}+\dot{r})^2}-\overbrace{V(q_{\rm cl})+rV'(q_{\rm cl})+\frac{r^2}{2}V''(q_{\rm cl})+\cdots}^{V(q_{\rm cl}+r)}\Big]$$

$$=S[q_{\rm cl}]+\int_0^t dt'r(t')\overbrace{\left[-m\ddot{q}_{\rm cl}-V'(q_{\rm cl})\right]}^{\frac{\delta S}{\delta q(t')}=0}+\frac{1}{2}\int_0^t dt'r(t')\overbrace{\left[-m\partial_{t'}^2-V''(q_{\rm cl})\right]}^{\frac{\delta^2 S}{\delta q(t')\delta q(t'')}}r(t')+\cdots$$

(ii) Classical trajectory: $m\ddot{q}_{\rm cl}=-V'(q_{\rm cl})$

Many solutions — choose non-singular solution $q_{\rm cl}=0$ *(why?)*

i.e. $S[q_{\rm cl}]=0$ and $V''(q_{\rm cl})=m\omega^2$ constant

$$G(0,0;t)\simeq\int_{r(0)=r(t)=0}Dr\exp\left[\frac{i}{\hbar}\int_0^t dt'r(t')\frac{m}{2}\left(-\partial_{t'}^2-\omega^2\right)r(t')\right]$$

N.B. if V was quadratic, expression trivially exact

More generally, $q_{\rm cl}(t)$ non-trivial $\mapsto$ non-vanishing $S[q_{\rm cl}]$ — see PS3

Fluctuation contribution? — example of a...

▷ Gaussian functional integration: *mathematical interlude*

- One variable Gaussian integral: $(\int_{-\infty}^{\infty} dv\, e^{-av^2/2})^2 = 2\pi \int_0^\infty r\, dr\, e^{-ar^2/2} = \frac{2\pi}{a}$

$$\int_{-\infty}^{\infty} dv\, e^{-\frac{a}{2}v^2} = \sqrt{\frac{2\pi}{a}}, \qquad \text{Re } a > 0$$

- More than one variable:

$$\int d\mathbf{v}\, e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}} = (2\pi)^{N/2} \det \mathbf{A}^{-1/2}$$

where $\mathbf{A}$ is +ve definite real symmetric $N \times N$ matrix

Proof: $\mathbf{A}$ diagonalised by orthogonal transformation: $\mathbf{A} = \mathbf{O}^T\mathbf{D}\mathbf{O}$

Change of variables: $\mathbf{w} = \mathbf{O}\mathbf{v}$ (Jacobian $\det(\mathbf{O}) = 1$) $\rightsquigarrow$ N decoupled Gaussian integrations: $\mathbf{v}^T\mathbf{A}\mathbf{v} = \mathbf{v}^T\mathbf{O}^T\mathbf{O}\mathbf{A}\mathbf{O}^T\mathbf{O}\mathbf{v} = \mathbf{w}^T\mathbf{D}\mathbf{w} = \sum_i^N d_i w_i^2$

Finally, $\prod_{i=1}^N d_i = \det \mathbf{D} = \det \mathbf{A}$

- Infinite number of variables; interpret $\{v_i\} \mapsto v(t)$ as continuous field and $A_{ij} \mapsto A(t,t') = \langle t|\hat{A}|t'\rangle$ as operator kernel

$$\int Dv(t)\, \exp\left[-\frac{1}{2}\int dt \int dt'\, v(t)A(t,t')v(t')\right] \propto (\det \hat{A})^{-1/2}$$

(iii) Applied to quantum well, $A(t,t') = -\frac{i}{\hbar}m\delta(t-t')(-\partial_{t'}^2 - \omega^2)$ and formally

$$G(0,0;t) \simeq J \det\left(-\partial_{t'}^2 - \omega^2\right)^{-1/2}$$

where J absorbs various constant prefactors ($im, \hbar$, etc.)

What does 'det' mean? Effectively, we have expanded trajectories $r(t')$ in eigenbasis of $\hat{A}$ subject to b.c. $r(t) = r(0) = 0$

$$\left(-\partial_t^2 - \omega^2\right) r_n(t) = \epsilon_n r_n(t), \qquad \text{cf. PIB}$$

i.e. Fourier series expn: $r_n(t') = \sin(\frac{n\pi t'}{t}), \quad n = 1, 2, \ldots, \qquad \epsilon_n = (\frac{n\pi}{t})^2 - \omega^2$

$$\det\left(-\partial_t^2 - \omega^2\right)^{-1/2} = \prod_{n=1}^{\infty} \epsilon_n^{-1/2} = \prod_{n=1}^{\infty} \left(\left(\frac{n\pi}{t}\right)^2 - \omega^2\right)^{-1/2}$$

▷ For $V = 0$, $G = G_{\text{free}}$ known — use to eliminate constant prefactor J

$$G(0,0;t) = \frac{G(0,0;t)}{G_{\text{free}}(0,0;t)} G_{\text{free}}(0,0;t) = \prod_{n=1}^{\infty}\left[1 - \left(\frac{\omega t}{n\pi}\right)^2\right]^{-1/2} \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \Theta(t)$$

Finally, applying identity $\prod_{n=1}^{\infty}[1 - (\frac{x}{n\pi})^2]^{-1} = \frac{x}{\sin x}$

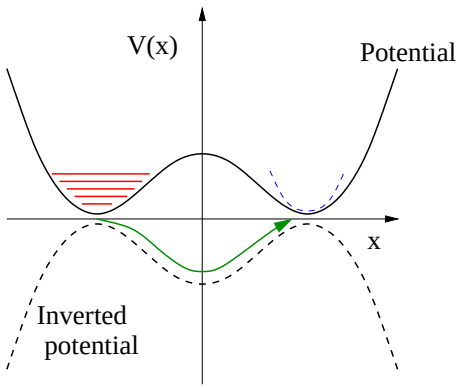
$$G(0,0;t) \simeq \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega t)}}\Theta(t)$$

(exact for harmonic oscillator)

Lecture XIII: Double Well Potential: Tunneling and Instantons

How can phenomena of QM tunneling be described by Feynman path integral?
No semi-classical expansion!

▷ E.g QM transition probability of particle in double well: $G(a,-a;t) \equiv \langle a|e^{-i\hat{H}t/\hbar}|-a\rangle$



▷ Feynman Path Integral:

$$G(a,-a;t) = \int_{q(0)=-a}^{q(t)=a} Dq \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(\frac{m}{2}\dot{q}^2 - V(q)\right)\right]$$

Stationary phase analysis: classical e.o.m. $m\ddot{q} = -\partial_q V$
$\mapsto$ only singular (high energy) solutions *Switch to alternative formulation...*

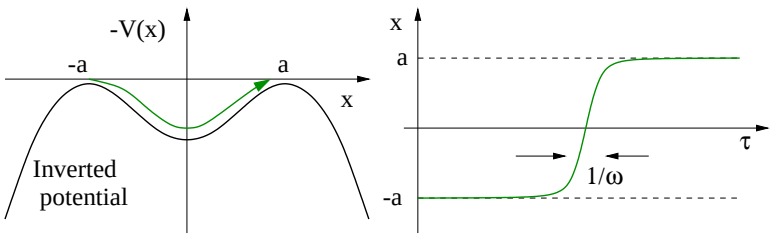
▷ Imaginary (Euclidean) time Path Integral: Wick rotation $t = -i\tau$
N.B. (relative) sign change! "$V \to -V$"

$$G(a,-a;\tau) = \int_{q(0)=-a}^{q(\tau)=a} Dq \exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' \left(\frac{m}{2}\dot{q}^2 + V(q)\right)\right]$$

Saddle-point analysis: classical e.o.m. $m\ddot{q} = +V'(q)$ in inverted potential!
solutions depend on b.c.

(1) $G(a,a;\tau) \rightsquigarrow q_{\rm cl}(\tau) = a$
(2) $G(-a,-a;\tau) \rightsquigarrow q_{\rm cl}(\tau) = -a$
(3) $G(a,-a;\tau) \rightsquigarrow q_{\rm cl}$: rolls from $-a$ to a

Combined with small fluctuations, (1) and (2) recover propagator for single well



(3) accounts for QM tunneling and is known as an "instanton" (or "kink")

▷ Instanton: classically forbidden trajectory connecting two degenerate minima
— i.e. topological, and therefore particle-like

For τ large, $\dot{q_{\rm cl}} \simeq 0$ (*evident*), i.e. "first integral" $m\dot{q_{\rm cl}}^2/2 - V(q_{\rm cl}) = \epsilon \overset{\tau\to\infty}{\to} 0$
precise value of ϵ fixed by b.c. (i.e. τ)

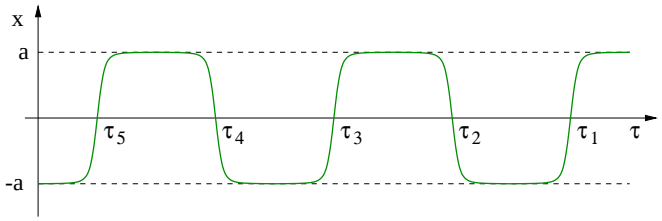
Saddle-point action *(cf. WKB $\int dqp(q)$)*

$$S_{\rm inst.} = \int_0^\tau d\tau' \left(\frac{m}{2}\dot{q}_{\rm cl}^2 + V(q_{\rm cl})\right) \simeq \int_0^\tau d\tau' m\dot{q}_{\rm cl}^2 = \int_{-a}^{a} dq_{\rm cl} m\dot{q}_{\rm cl} = \int_{-a}^{a} dq_{\rm cl}(2mV(q_{\rm cl}))^{1/2}$$

Structure of instanton: For $q \simeq a$, $V(q) = \frac{1}{2}m\omega^2(q-a)^2 + \cdots$, i.e. $\dot{q}_{\rm cl} \overset{\tau\to\infty}{\simeq} \omega(q_{\rm cl} - a)$

$q_{\rm cl}(\tau) \overset{\tau\to\infty}{=} a - e^{-\tau\omega}$, i.e. temporal extension set by $\omega^{-1} \ll \tau$

Imples existence of approximate saddle-point solutions
involving many instantons (and anti-instantons): instanton gas



▷ Accounting for fluctuations around n-instanton configuration

$$G(a, \pm a; \tau) \simeq \sum_{n \text{ even / odd}} K^n \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n \overbrace{A_n(\tau_1, \ldots, \tau_n)}^{A_{n,\rm cl.}A_{n,\rm qu.}},$$

constant K set by normalisation

$A_{n,\rm cl.} = e^{-nS_{\rm inst.}/\hbar}$ — 'classical' contribution

$A_{n,\rm qu.}$ — quantum fluctuations (imported from single well): $G_{\rm s.w.}(0,0;t) \sim \frac{1}{\sqrt{\sin\omega t}}$

$$A_{n,\rm qu.} \sim \prod_i^n \frac{1}{\sqrt{\sin(-i\omega(\tau_{i+1} - \tau_i))}} \sim \prod_i^n e^{-\omega(\tau_{i+1}-\tau_i)/2} \sim e^{-\omega\tau/2}$$

$$G(a, \pm a; \tau) \simeq \sum_{n \text{ even / odd}} K^n e^{-nS_{\rm inst.}/\hbar} e^{-\omega\tau/2} \overbrace{\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n}^{\tau^n/n!}$$

$$= \sum_{n \text{ even / odd}} e^{-\omega\tau/2} \frac{1}{n!} \left(\tau K e^{-S_{\rm inst.}/\hbar}\right)^n$$

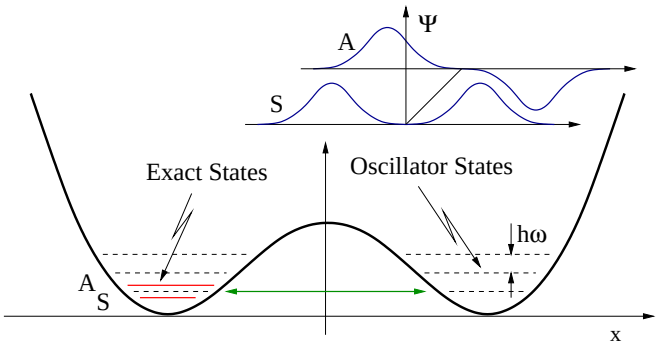
Using $e^x = \sum_{n=0}^\infty x^n/n!$, N.B. non-perturbative in $\hbar$!

$$\begin{aligned} G(a, a; \tau) &\simeq Ce^{-\omega\tau/2} \cosh\left(\tau K e^{-S_{\rm inst.}/\hbar}\right) \\ G(a, -a; \tau) &\simeq Ce^{-\omega\tau/2} \sinh\left(\tau K e^{-S_{\rm inst.}/\hbar}\right) \end{aligned}$$

Consistency check: main contribution from

$$\bar{n} = \langle n \rangle \equiv \frac{\sum_n n X^n/n!}{\sum_n X^n/n!} = X = \tau K e^{-S_{\rm inst.}/\hbar}$$

no. per unit time, $\bar{n}/\tau$ exponentially small, and indep. of τ, i.e. dilute gas



▷ Physical interpretation: For infinite barrier — two independent oscillators,
coupling splits degeneracy — symmetric/antisymmetric

$$G(a, \pm a; \tau) \simeq \langle a|S\rangle e^{-\epsilon_S \tau/\hbar} \langle S| \pm a\rangle + \langle a|A\rangle e^{-\epsilon_A \tau/\hbar} \langle A| \pm a\rangle$$

$$|\langle a|S\rangle|^2 = \langle a|S\rangle\langle S| - a\rangle = \frac{C}{2}, \qquad |\langle a|A\rangle|^2 = -\langle a|A\rangle\langle A| - a\rangle = \frac{C}{2}$$

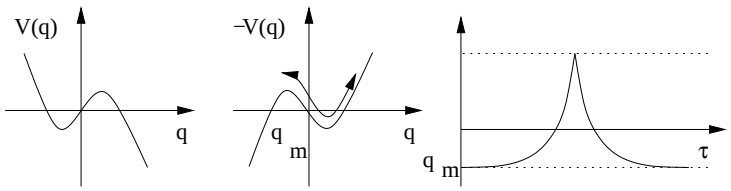
Setting: $\epsilon_{A/S} = \hbar\omega/2 \pm \Delta\epsilon/2$

$$G(a, \pm a; \tau) \simeq \frac{C}{2}\left(e^{-(\hbar\omega - \Delta\epsilon)\tau/2\hbar} \pm e^{-(\hbar\omega + \Delta\epsilon)\tau/2\hbar}\right) = C e^{-\omega\tau/2} \begin{cases} \cosh(\Delta\epsilon\tau/\hbar) \\ \sinh(\Delta\epsilon\tau/\hbar) \end{cases} .$$

▷ Remarks:

(i) Legitimacy? How do (neglected) terms $O(\hbar^2)$ compare to $\Delta\epsilon$?

In fact, such corrections are bigger but act equally on $|S\rangle$ and $|A\rangle$
i.e. $\Delta\epsilon = \hbar K e^{-S_{\rm inst.}/\hbar}$ is dominant contribution to splitting



(ii) Unstable States and Bounces: survival probability: $G(0,0;t)$? No even/odd effect:

$$G(0,0;\tau) = C e^{-\omega\tau/2} \exp\left[\tau K e^{-S_{\rm inst}/\hbar}\right] \stackrel{\tau = it}{=} C e^{-i\omega t/2} \exp\left[-\frac{\Gamma}{2} t\right]$$

Decay rate: $\Gamma \sim |K| e^{-S_{\rm inst}/\hbar}$ (i.e. K imaginary) *N.B. factor of* 2

Lecture XIV: Coherent States

Discuss element of PI construction which demands generalisation

▷ Generalisation of FPI to many-body systems problematic
due to particle indistinguishability and statistics

Can second quantisation help? *automatically respects particle statistics*

Require complete basis on the Fock space to construct PI

Such eigenstates exist and are known as Coherent States
reference: Negele and Orland

▷ Coherent States (Bosons)

What are eigenstates of Fock space operators: a_i and $a_i^\dagger$ s.t. $[a_i, a_j^\dagger] = \delta_{ij}$?

Being a state of the Fock space, an eigenstate $|\phi\rangle$ can be expanded as

$$|\phi\rangle = \sum_{n_1,n_2,\cdots} C_{n_1,n_2,\cdots} \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1}} \frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2}} \cdots |0\rangle$$

N.B. notation $|0\rangle$ for vacuum state!

(i) $a_i^\dagger|\phi\rangle = \phi_i|\phi\rangle$? — in fact, eigenstate of $a_i^\dagger$ can not exist:
if the minimum occupation of $|\phi\rangle$ is n_0, the minimum of $a_i^\dagger|\phi\rangle$ is $n_0 + 1$

(ii) $a_i|\phi\rangle = \phi_i|\phi\rangle$? — can exist and given by: $\boxed{|\phi\rangle \equiv \exp[\sum_i \phi_i a_i^\dagger]|0\rangle}$ N.B. $\phi \equiv \{\phi_i\}$

Proof: *since a_i commutes with all $a_j^\dagger$ for $j \neq i$ — focus on one element i*

$$a \exp(\phi a^\dagger)|0\rangle = [a, \exp(\phi a^\dagger)]|0\rangle =$$
$$= \sum_{n=0}^{\infty} \frac{\phi^n}{n!}[a, (a^\dagger)^n]|0\rangle = \sum_{n=1}^{\infty} \frac{n\phi^n}{n!}(a^\dagger)^{n-1}|0\rangle = \phi \exp(\phi a^\dagger)|0\rangle$$

$$a(a^\dagger)^n = aa^\dagger(a^\dagger)^{n-1} = (1 + a^\dagger a)(a^\dagger)^{n-1} = (a^\dagger)^{n-1} + a^\dagger a(a^\dagger)^{n-1} = n(a^\dagger)^{n-1} + (a^\dagger)^n a$$

i.e. $|\phi\rangle$ is eigenstate of all a_i with eigenvalue ϕ_i — known as Bosonic coherent state

▷ Properties of coherent state:

- Hermitian conjugation:

$$\forall i: \quad \langle\phi|a_i^\dagger = \langle\phi|\bar{\phi}_i$$

$\bar{\phi}_i$ is complex conjugate of ϕ_i

- By direct application of ∂_{ϕ_i} (and operator commutativity):

$$\forall i: \quad a_i^\dagger|\phi\rangle = \partial_{\phi_i}|\phi\rangle$$

- Overlap: with $\langle\theta| = (|\theta\rangle)^\dagger = \langle 0|e^{\sum_i \bar{\theta}_i a_i}$

$$\langle\theta|\phi\rangle = \langle 0|e^{\sum_i \bar{\theta}_i a_i}|\phi\rangle = e^{\sum_i \bar{\theta}_i \phi_i}\langle 0|\phi\rangle = \exp\left[\sum_i \bar{\theta}_i\phi_i\right]$$

i.e. states are not orthogonal! *operators not Hermitian*

- Norm: $\langle\phi|\phi\rangle = \exp\left[\sum_i \bar{\phi}_i\phi_i\right]$

- Completeness — resolution of id. (for proof see notes)

$$\boxed{\int \prod_i \frac{d\bar{\phi}_i d\phi_i}{\pi} e^{-\sum_i \bar{\phi}_i\phi_i}|\phi\rangle\langle\phi| = \mathbf{1}_{\mathcal{F}}}$$

where $d\bar{\phi}_i d\phi_i = d\mathrm{Re}\,\phi_i d\mathrm{Im}\,\phi_i$

▷ Coherent States (Fermions)

Following bosonic case, seek state $|\eta\rangle$ s.t.

$$a_i|\eta\rangle = \eta_i|\eta\rangle, \qquad \eta = \{\eta_i\}$$

But anticommutativity $[a_i, a_j]_+ = 0$ $(i \neq j)$ implies eigenvalues η_i anticommute!!

$$\eta_i\eta_j = -\eta_j\eta_i$$

η_i can not be ordinary numbers — in fact, they obey...

▷ Grassmann Algebra

In addition to anticommutativity, defining properties:

(i) $\eta_i^2 = 0$ (cf. fermions) but note: these are not operators, i.e. $[\eta_i, \bar{\eta}_i]_+ \neq 1$

(ii) Elements η_i can be added to and multiplied by ordinary complex numbers

$$c + c_i\eta_i + c_j\eta_j, \quad c_i, c_j \in \mathcal{C}$$

(iii) Grassmann numbers anticommute with fermionic creation/annihilation operators

$$[\eta_i, a_j]_+ = 0$$

▷ Calculus of Grassmann variables:

(iv) Differentiation: $\partial_{\eta_i}\eta_j = \delta_{ij}$

N.B. ordering $\partial_{\eta_i}\eta_j\eta_i = -\eta_j\partial_{\eta_i}\eta_i = -\eta_j$ for $i \neq j$

(v) Integration: $\int d\eta_i = 0, \quad \int d\eta_i \eta_i = 1$
i.e. differentiation and integration have the same effect!!

▷ Gaussian integration:

$$\int d\bar{\eta} d\eta \, e^{-\bar{\eta} a \eta} = \int d\bar{\eta} d\eta \, (1 - \bar{\eta} a \eta) = a \int d\bar{\eta} \bar{\eta} \int d\eta \eta = a$$

$$\int d\bar{\eta} d\eta \, e^{-\bar{\eta}^T \mathbf{A} \eta} = \det \mathbf{A} \qquad \text{(exercise)}$$

cf. ordinary complex variables

▷ Functions of Grassmann variables:

Taylor expansion terminates at low order since $\eta^2 = 0$, e.g.

$$F(\eta) = F(0) + \eta F'(0)$$

Using rules

$$\int d\eta F(\eta) = \int d\eta \, [F(0) + \eta F'(0)] = F'(0) \equiv \partial_\eta F[\eta]$$

i.e. differentiation and integration have same effect on $F[\eta]$!

Usually, one has a function of many variables $F[\eta]$, say $\eta = \{\eta_1, \cdots \eta_N\}$

$$F(\eta) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n F(0)}{\partial \eta_i \cdots \partial \eta_j} \eta_j \cdots \eta_i$$

but series must terminate at $n = N$

with these preliminaries we are in a position to introduce the

▷ Fermionic coherent state: $\boxed{|\eta\rangle = \exp[-\sum_i \eta_i a_i^\dagger]|0\rangle}$ i.e. $\eta = \{\eta_i\}$

Proof (cf. bosonic case)

$$a \exp(-\eta a^\dagger)|0\rangle = a(1 - \eta a^\dagger)|0\rangle = \eta a a^\dagger |0\rangle = \eta |0\rangle = \eta \exp(-\eta a^\dagger)|0\rangle$$

Other defining properties mirror bosonic CS — *problem set*

▷ Differences:

(i) Adjoint: $\langle \eta| = \langle 0| e^{-\sum_i a_i \bar{\eta}_i} \equiv \langle 0| e^{\sum_i \bar{\eta}_i a_i}$ but N.B. $\bar{\eta}_i$ not related to η_i!

(ii) Gaussian integration: $\int d\bar{\eta} d\eta \, e^{-\bar{\eta}\eta} = 1$ N.B. no π's

Completeness relation

$$\boxed{\int \prod_i d\bar{\eta}_i d\eta_i e^{-\sum_i \bar{\eta}_i \eta_i} |\eta\rangle\langle\eta| = \mathbf{1}_F}$$

Lecture XV: Many-body (Coherent State) Path Integral

Could formulate many-body propagator (Green function), but here, convenient to focus on partition function.

▷ Quantum partition function

$$\mathcal{Z} = \sum_{\{n\}\in\text{Fock Space}} \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle, \qquad \beta = 1/k_BT, \qquad \mu \text{ chemical potential}$$

Coherent state representation of $\mathcal{Z}$ — insert resolution of id. (fermions/bosons)

$$\int d[\bar{\psi},\psi]e^{-\sum_i \bar{\psi}_i\psi_i}|\psi\rangle\langle\psi| = \mathbf{1}_{\mathcal{F}}, \qquad d[\bar{\psi},\psi] \equiv \prod_i \frac{d\bar{\psi}_i d\psi_i}{\pi^{(1-\zeta)/2}}$$

each element ψ_i associated with one basis state, viz. $a_i^\dagger$
— e.g. i may include position, momentum, spin, lattice site, etc.

$$\mathcal{Z} = \int d[\bar{\psi},\psi]e^{-\sum_i \bar{\psi}_i\psi_i}\sum_n \langle n|\psi\rangle\langle\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle$$

Elimination of $|n\rangle$ requires identity: $\langle n|\psi\rangle\langle\psi|n\rangle = \langle -\zeta\psi|n\rangle\langle n|\psi\rangle$

Proof: E.g. $|n\rangle = a_1^\dagger a_2^\dagger\cdots a_n^\dagger|0\rangle$

$$\begin{aligned}
\langle n|\psi\rangle &= \langle 0|a_n\cdots a_2a_1|\psi\rangle = \psi_n\cdots\psi_2\psi_1\langle 0|\psi\rangle = \psi_n\cdots\psi_2\psi_1 \\
\langle\psi|n\rangle &= \bar{\psi}_1\bar{\psi}_2\cdots\bar{\psi}_n \\
\langle n|\psi\rangle\langle\psi|n\rangle &= \psi_n\cdots\psi_2\psi_1\bar{\psi}_1\bar{\psi}_2\cdots\bar{\psi}_n = \psi_1\bar{\psi}_1\psi_2\bar{\psi}_2\cdots\psi_n\bar{\psi}_n \\
&= (-\zeta\bar{\psi}_1\psi_1)(-\zeta\bar{\psi}_2\psi_2)\cdots(-\zeta\bar{\psi}_n\psi_n) = \langle -\zeta\psi|n\rangle\langle n|\psi\rangle
\end{aligned}$$

commute through and erase $\sum_n |n\rangle\langle n|$

$$\boxed{\mathcal{Z} = \int d[\bar{\psi},\psi]e^{-\sum_i \bar{\psi}_i\psi_i}\langle -\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle}$$

▷ Coherent State Path Integral

Applied to general Hamiltonian

$$\hat{H}-\mu\hat{N} = \sum_{ij}(h_{ij}-\mu\delta_{ij})a_i^\dagger a_j + \sum_{ijkl} V_{ijkl}a_i^\dagger a_j^\dagger a_k a_l$$

N.B. operators are normal ordered

Follow general strategy of Feynman:

(i) Divide 'time interval' β into N segments $\Delta\beta = \beta/N$

$$\langle -\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle = \langle -\zeta\psi|e^{-\Delta\beta(\hat{H}-\mu\hat{N})}\wedge e^{-\Delta\beta(\hat{H}-\mu\hat{N})}\wedge\cdots|\psi\rangle$$

(ii) At each $\wedge$ insert resolution of id.

$$\mathbf{1}_{\mathcal{F}} = \int d[\bar{\psi}_n,\psi_n]e^{-\bar{\psi}_n\cdot\psi_n}|\psi_n\rangle\langle\psi_n|$$

i.e. N-independent sets N.B. each ψ_n is a vector with elements $\{\psi_i\}_n$

(iii) Expand exponent in $\Delta\beta$

$$\begin{aligned}\langle\psi'|e^{-\Delta\beta(\hat{H}-\mu\hat{N})}|\psi\rangle &= \langle\psi'|\left[1-\Delta\beta(\hat{H}-\mu\hat{N})\right]|\psi\rangle + O(\Delta\beta)^2\\ &= \langle\psi'|\psi\rangle - \Delta\beta\langle\psi'|(\hat{H}-\mu\hat{N})|\psi\rangle + O(\Delta\beta)^2\\ &= \langle\psi'|\psi\rangle\left[1-\Delta\beta\left(H(\psi',\psi)-\mu N(\psi',\psi)\right)\right] + O(\Delta\beta)^2\\ &\simeq e^{\psi'\cdot\psi}e^{-\Delta\beta(H(\psi',\psi)-\mu N(\psi',\psi))}\end{aligned}$$

$$\text{with}\qquad H(\psi',\psi) = \frac{\langle\psi'|\hat{H}|\psi\rangle}{\langle\psi'|\psi\rangle} = \sum_{ij}h_{ij}\bar{\psi}'_i\psi_j + \sum_{ijkl}V_{ijkl}\bar{\psi}'_i\bar{\psi}'_j\psi_k\psi_l$$

similarly $N(\psi',\psi)$ *N.B. $\langle\psi'|\psi\rangle$ bilinear in ψ, i.e. commutes with everything*

$$\mathcal{Z} = \int_{\bar{\psi}_N=-\zeta\bar{\psi}_0,\psi_N=-\zeta\psi_0}\prod_{n=0}^{N} d[\bar{\psi}_n,\psi_n]e^{-\sum_{n=1}^{N}\left[\bar{\psi}_n\cdot(\psi_n-\psi_{n-1})+\Delta\beta(H(\bar{\psi}_n,\psi_{n-1})-\mu N(\bar{\psi}_n,\psi_{n-1}))\right]}$$

Continuum limit $N\to\infty$

$$\Delta\beta\sum_{n=0}^{N}\to\int_0^\beta d\tau,\qquad \frac{\psi_n-\psi_{n-1}}{\Delta\beta}\to\partial_\tau\psi\Big|_{\tau=n\Delta\beta},\qquad \prod_{n=0}^{N}d[\bar{\psi}_n,\psi_n]\to D(\bar{\psi},\psi)$$

comment on "small" Grassmann nos.

$$\boxed{\mathcal{Z} = \int_{\substack{\bar{\psi}(\beta)=-\zeta\bar{\psi}(0)\\ \psi(\beta)=-\zeta\psi(0)}} D(\bar{\psi},\psi)e^{-S[\bar{\psi},\psi]},\qquad S[\bar{\psi},\psi] = \int_0^\beta d\tau\left(\bar{\psi}\cdot\partial_\tau\psi + H(\bar{\psi},\psi) - \mu N(\bar{\psi},\psi)\right)}$$

With particular example:

$$S[\bar{\psi},\psi] = \int_0^\beta d\tau\left[\sum_{ij}\bar{\psi}_i(\tau)\left[(\partial_\tau-\mu)\delta_{ij}+h_{ij}\right]\psi_j(\tau) + \sum_{ijkl}V_{ijkl}\,\bar{\psi}_i(\tau)\bar{\psi}_j(\tau)\psi_k(\tau)\psi_l(\tau)\right]$$

i.e. Quantum partition function expressed as path integral over fields $\psi_j(\tau)$

▷ Matsubara frequency representation

Often convenient to express path integral in frequency domain

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} \psi_n e^{i\omega_n \tau}, \qquad \psi_{\omega_n} = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau\, \psi(\tau) e^{-i\omega_n \tau}$$

where, since $\psi(\tau) = -\zeta\psi(\tau+\beta)$

$$\omega_n = \begin{cases} 2n\pi/\beta, & \text{bosons,} \\ (2n+1)\pi/\beta, & \text{fermions} \end{cases}, \quad n \in \mathcal{Z}$$

ω_n are known as Matsubara frequencies

Using $\dfrac{1}{\beta}\displaystyle\int_0^\beta d\tau\; e^{i(\omega_n - \omega_m)\tau} = \delta_{\omega_n \omega_m}$

$$S[\bar{\psi}, \psi] = \sum_{ij\omega_n} \bar{\psi}_{i\omega_n} \left[(i\omega_n - \mu)\, \delta_{ij} + h_{ij} \right] \psi_{j\omega_n} +$$

$$+ \frac{1}{\beta} \sum_{ijkl} \sum_{\omega_{n_1} \omega_{n_2} \omega_{n_3} \omega_{n_4}} V_{ijkl} \bar{\psi}_{i\omega_{n_1}} \bar{\psi}_{j\omega_{n_2}} \psi_{k\omega_{n_3}} \psi_{l\omega_{n_4}} \delta_{\omega_{n_1} + \omega_{n_2}, \omega_{n_3} + \omega_{n_4}}$$

Lecture XVI: Applications and Connections

▷ Partition Function of ideal (Non-Interacting) Gas of Quantum Particles

Useful for "normalisation" of interacting theories

e.g. Non-interacting fermions: $\hat{H} = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha$

As a warm-up exercise, let us first use coherent state representation:

Quantum Partition function

$$\mathcal{Z}_0 = \text{tr } e^{-\beta(\hat{H}-\mu\hat{N})} = \sum_n \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle$$

In coherent state basis:

$$\mathcal{Z}_0 = \int d[\bar{\psi},\psi] e^{-\sum_\alpha \bar{\psi}_\alpha\psi_\alpha} \langle -\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle$$

Using ident. *N.B.* $\hat{n}_\alpha^2 = \hat{n}_\alpha$

$$e^{-\beta(\hat{H}-\mu\hat{N})} = e^{-\beta\sum_\alpha(\epsilon_\alpha-\mu)a_\alpha^\dagger a_\alpha} = \prod_\alpha e^{-\beta(\epsilon_\alpha-\mu)\hat{n}_\alpha} = \prod_\alpha \left[1 + \left(e^{-\beta(\epsilon_\alpha-\mu)} - 1\right)\hat{n}_\alpha\right]$$

$$\begin{aligned}
\mathcal{Z}_0 &= \int d[\bar{\psi},\psi] e^{-\sum_\alpha \bar{\psi}_\alpha\psi_\alpha} \prod_\alpha \Big\{ \overbrace{e^{-\bar{\psi}_\alpha\psi_\alpha}}^{\langle -\psi|\psi\rangle} \left[1 + \left(e^{-\beta(\epsilon_\alpha-\mu)} - 1\right)(-\bar{\psi}_\alpha\psi_\alpha)\right] \Big\} \\
&= \prod_\alpha \int d\bar{\psi}_\alpha d\psi_\alpha \ \overbrace{e^{-2\bar{\psi}_\alpha\psi_\alpha}}^{1-2\bar{\psi}_\alpha\psi_\alpha} \left[1 + \left(e^{-\beta(\epsilon_\alpha-\mu)} - 1\right)(-\bar{\psi}_\alpha\psi_\alpha)\right] \\
&= \prod_\alpha \int d\bar{\psi}_\alpha d\psi_\alpha \ \left[1 - 2\bar{\psi}_\alpha\psi_\alpha - \left(e^{-\beta(\epsilon_\alpha-\mu)} - 1\right)\bar{\psi}_\alpha\psi_\alpha\right] \\
&= \prod_\alpha \int d\bar{\psi}_\alpha d\psi_\alpha \ \left[-\bar{\psi}_\alpha\psi_\alpha(1 + e^{-\beta(\epsilon_\alpha-\mu)})\right] \\
&= \prod_\alpha \left[1 + e^{-\beta(\epsilon_\alpha-\mu)}\right] \qquad \text{i.e. Fermi} - \text{Dirac distribution}
\end{aligned}$$

Exercise: show (using CS) that in Bosonic case

$$\mathcal{Z}_0 = \prod_\alpha \sum_{n=0}^\infty e^{-n\beta(\epsilon_\alpha-\mu)} = \prod_\alpha \left[1 - e^{-\beta(\epsilon_\alpha-\mu)}\right]^{-1}$$

Bose-Einstein distribution

▷ Connection of CSPI with FPI

e.g. Quantum Harmonic oscillator: $\hat{H} = \dfrac{\hat{p}^2}{2m} + \dfrac{1}{2}m\omega^2\hat{q}^2$

In second quantised form, $\hat{H} = (a^\dagger a + 1/2)\hbar\omega, \qquad [a, a^\dagger] = 1$, i.e. bosons!

$$\mathcal{Z} = \mathrm{tr}(e^{-\beta\hat{H}}) = \int_{\psi(\beta)=\psi(0)}^{\bar{\psi}(\beta)=\bar{\psi}(0)} D[\bar{\psi},\psi] \exp\left[-\int_0^\beta \left(\bar{\psi}\partial_\tau\psi + \hbar\omega\bar{\psi}\psi\right)\right]$$

$e^{-\beta\hbar\omega/2}$ *in* $D[\bar{\psi},\psi]$, $\psi(\tau)$ — complex scalar field

Parameterise complex field in terms of two real scalar fields

$$\psi(\tau) = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left[q(\tau) + \frac{ip(\tau)}{m\omega}\right]$$

Substituting (e.g. $\hbar\omega\bar{\psi}\psi = \frac{m\omega^2}{2}(q^2 + \frac{p^2}{(m\omega)^2})$) and noting $\displaystyle\int_0^\beta d\tau\, q\dot{p} = -\int_0^\beta d\tau\, p\dot{q}$

$$\mathcal{Z} = \int_{\psi(\beta)=\psi(0)}^{\bar{\psi}(\beta)=\bar{\psi}(0)} D[p,q] \exp\left[-\int_0^\beta d\tau \left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 - \frac{ip\dot{q}}{\hbar}\right)\right]$$

cf. (Euclidean time) FPI $\beta = it/\hbar$, $\tau = it'/\hbar$, $\frac{i}{\hbar}\frac{\partial q}{\partial\tau} = \frac{\partial q}{\partial t'}$

$$\mathcal{Z} = \int D[p,q] \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(p\dot{q} - H(p,q)\right)\right]$$

Partition Function of Harmonic Oscillator from CSPI

(i) Bosonic oscillator:

$$\mathcal{Z}_B = \overbrace{\int D[\bar{\psi},\psi] \exp\left[-\int_0^\beta d\tau \bar{\psi}\left(\partial_\tau + \hbar\omega\right)\psi\right]}^{J\det(\partial_\tau+\hbar\omega)^{-1}} = \int (\prod_n d\bar{\psi}_{\omega_n} d\psi_{\omega_n}) e^{-\sum_n \bar{\psi}_{\omega_n}(i\omega_n+\hbar\omega)\psi_{\omega_n}}$$

$$= J\prod_{\omega_n}\left[i\omega_n + \hbar\omega\right]^{-1} = \frac{J}{\hbar\omega}\prod_{n=1}^\infty\left[(\hbar\omega)^2 + \left(\frac{2n\pi}{\beta}\right)^2\right]^{-1} \frac{J'}{\hbar\omega}\prod_{n=1}^\infty\left[1 + \left(\frac{\hbar\omega\beta}{2\pi n}\right)^2\right]^{-1}$$

$$= \frac{J'}{2\beta\sinh(\hbar\omega\beta/2)}$$

$\prod_{n=1}^\infty[1 + (x/\pi n)^2] = (\sinh x)/x$

Normalisation: $T \to 0$, $\mathcal{Z}$ dominated by g.s. $\lim_{\beta\to\infty}\mathcal{Z}_B = e^{-\beta\hbar\omega/2} (= \mathcal{Z}_F)$

$$\text{i.e. } J' = \beta \qquad \mathcal{Z}_B = \frac{1}{2\sinh(\hbar\beta\omega/2)}$$

(ii) Fermionic oscillator: Gaussian Grassmann integration

$$\begin{aligned}\mathcal{Z}_F &= J\det(\partial_\tau + \hbar\omega) = J\prod_{\omega_n}[i\omega_n + \hbar\omega] = J\prod_{n=0}^{\infty}\left[(\hbar\omega)^2 + \left(\frac{(2n+1)\pi}{\beta}\right)^2\right] \\ &= J'\prod_{n=1}^{\infty}\left[1 + \left(\frac{\hbar\omega\beta}{(2n+1)\pi}\right)^2\right] = J'\cosh(\hbar\omega\beta/2)\end{aligned}$$

$$\textstyle\prod_{n=1}^{\infty}[1 + (x/\pi(2n+1))^2] = \cosh(x/2)$$

Using normalisation: $\lim_{\beta\to\infty}\mathcal{Z}_F = e^{-\beta\hbar\omega/2}$

$$J' = 2e^{-\beta\hbar\omega} \qquad \mathcal{Z}_F = 2e^{-\beta\hbar\omega}\cosh(\hbar\beta\omega/2).$$

cf. direct computation:

$$\mathcal{Z}_B = e^{-\beta\hbar\omega/2}\sum_{n=0}^{\infty}e^{-n\beta\hbar\omega}, \qquad \mathcal{Z}_F = e^{-\beta\hbar\omega/2}\sum_{n=0}^{1}e^{-n\beta\hbar\omega}.$$

Note that normalising prefactor J' involves only a constant offset of free energy,

$$F = -k_{\rm B}T\ln\mathcal{Z}$$

statistical correlations encoded in content of functional integral

▷ *In notes, two case studies:*

(i) Plasma Theory of the weakly interacting electron gas

(ii) BCS theory of superconductivity — a prototype for gauge theories

We will deal with project (ii)

Lecture XVII: Weakly Interacting Electron Gas: Plasma Theory

▷ How are the properties of an electron gas influenced by weak Coulomb interaction?

▷ QUALITATIVE CONSIDERATIONS:

When is the intereaction weak? Defining $r_0 = \frac{1}{n^{1/3}}$ as the average electron separation, the typical p.e. $\frac{e^2}{r_0}$ and k.e. $\frac{\hbar^2}{mr_0}$ lead to the dimensionless ratio, $r_s = \dfrac{e^2}{r_0}\dfrac{mr_0^2}{\hbar^2} \equiv \dfrac{r_0}{a_0}$, where a_0 is electron Bohr radius, from which one can infer that Coulomb effects dominate at low density

At $r_s \sim 35$ there is (believed to be) a transition to an electron solid phase known as a Wigner crystal (cf. Mott-Hubbard insulator)

For most metals ($2 < r_s < 6$), k.e. and p.e. comparable; fortunately (thanks to adiabatic continuity) "weak coupling" theory valid even for intermediate r_s

▷ Motivates consideration of weak coupling theory $r_s \ll 1$: Σ-convention on spin

$$\hat{H} = \int d^d r\, c_\sigma^\dagger(\mathbf{r}) \frac{\hat{\mathbf{p}}^2}{2m} c_\sigma(\mathbf{r}) + \frac{1}{2}\int d^d r \int d^d r' c_\sigma^\dagger(\mathbf{r}) c_{\sigma'}^\dagger(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} c_{\sigma'}(\mathbf{r}') c_\sigma(\mathbf{r})$$

Aim: to explore dielectric properties and ground state energy of electron gas through...

▷ QUANTUM PARTITION FUNCTION: using CSPI formulation

$$\mathcal{Z} \equiv \text{tr}\; e^{-\beta(\hat{H}-\mu\hat{N})} = \int_{\substack{\bar{\psi}_\sigma(0)=-\bar{\psi}_\sigma(\beta) \\ \psi_\sigma(0)=-\psi_\sigma(\beta)}} D(\bar{\psi}_\sigma, \psi_\sigma) e^{-S[\bar{\psi}_\sigma, \psi_\sigma]}$$

$$S[\bar{\psi}_\sigma, \psi_\sigma] = \int_0^\beta d\tau \left[\int d^d r\, \bar{\psi}_\sigma(\mathbf{r},\tau) \left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu \right) \psi_\sigma(\mathbf{r},\tau) \right.$$
$$\left. + \frac{1}{2}\int d^d r \int d^d r' \bar{\psi}_\sigma(\mathbf{r},\tau) \bar{\psi}_{\sigma'}(\mathbf{r}',\tau) \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \psi_{\sigma'}(\mathbf{r}',\tau) \psi_\sigma(\mathbf{r},\tau) \right]$$

Expressed in Fourier basis: $\psi_\sigma(\mathbf{r},\tau) = \dfrac{1}{\sqrt{L^3\beta}} \sum_{\mathbf{k},\omega_n} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_n\tau)} \psi_{\mathbf{k},\omega_n,\sigma}$

$$S = \int_0^\beta d\tau \left[\sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}\sigma}(\tau) \left(\partial_\tau + \epsilon_{\mathbf{k}} - \mu \right) \psi_{\mathbf{k}\sigma}(\tau) + \frac{1}{2L^d} \sum_{\mathbf{q}\neq 0} \frac{4\pi e^2}{\mathbf{q}^2} \rho_{\mathbf{q}}(\tau) \rho_{-\mathbf{q}}(\tau) \right]$$

where $\epsilon_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2m}$ and $\rho_{\mathbf{q}}(\tau) = \int d^d r\, e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r},\tau) \equiv \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}\sigma}(\tau) \psi_{\mathbf{k}+\mathbf{q},\sigma}(\tau)$
(N.B. neutralising background $\rightsquigarrow$ exclusion of $\mathbf{q} = 0$ from sum)

With the action quartic in fermionic fields ψ, $\mathcal{Z}$ can not be evaluated exactly

For weak interaction, $r_s \ll 1$, we could expand in Coulomb interaction:
$\rightsquigarrow$ Feynman diagram expansion (cf. Gell-Mann—Brückner theory)

Alternative — use field integral to isolate leading diagrammatic series expansion
— known as the Random Phase Approximation (RPA)

▷ General principle:

When confronted with interacting field theory, seek decomposition of interaction through introduction of auxiliary field which captures low-energy content of theory

In some cases, these fields are identified with the elementary particles that mediate the interaction (see below); in others, these fields encode the low-energy collective modes of the system (e.g. superfluid, superconductor)

▷ Decoupling facilitated using the Hubbard-Stratonovich transformation:

$$e^{-\int_0^\beta d\tau \sum_{\mathbf{q}\neq 0} \frac{2\pi e^2}{L^d \mathbf{q}^2} \rho_{\mathbf{q}}(\tau)\rho_{-\mathbf{q}}(\tau)} = \int D\phi \; e^{-\int_0^\beta d\tau \sum_{\mathbf{q}\neq 0} \left[\frac{\mathbf{q}^2}{8\pi}\phi_{\mathbf{q}}(\tau)\phi_{-\mathbf{q}}(\tau) + \frac{ie}{2L^{d/2}}(\phi_{\mathbf{q}}(\tau)\rho_{-\mathbf{q}}(\tau)+\rho_{\mathbf{q}}(\tau)\phi_{-\mathbf{q}}(\tau))\right]}$$

▷ Physically, ϕ represents (scalar) photon field which mediates Coulomb interaction
N.B. ϕ real and periodic $\phi(\tau+\beta)=\phi(\tau)$

$$\mathcal{Z} = \int D(\bar{\psi}_\sigma, \psi_\sigma) \int D\phi \; \exp\left\{ -\int_0^\beta d\tau \int d^d r \left[\frac{1}{8\pi}(\partial\phi)^2 + \bar{\psi}_\sigma \left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi \right) \psi_\sigma \right] \right\}$$

Gaussian in Grassmann fields, field integral may be performed:
using identity $\int D[\bar{\psi},\psi]\exp[-\bar{\psi}M\psi] = \det M = \exp[\ln\det M]$

$$\boxed{\mathcal{Z} = \int D\phi \exp\Big[-\int_0^\beta d\tau \int d^d r \frac{1}{8\pi}(\partial\phi)^2 + \overbrace{2}^{\text{spin}} \ln\det\left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi \right) \Big]}$$

Setting $e=0$, photon field decouples from determinant;
recovers partition function of non-interacting electron gas

▷ Perturbation Theory in e:

Define free particle Green function: $\hat{G}_0 = [\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu]^{-1}$ and expand:
$\ln(1+x) = -\sum_{n=1}(-x)^n/n$

$$\begin{aligned} \ln\det\left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi \right) &\equiv \operatorname{tr}\ln\left(\hat{G}_0^{-1} + ie\phi \right) = \operatorname{tr}\ln\hat{G}_0^{-1} + \operatorname{tr}\ln\left[1 + ie\hat{G}_0\phi \right] \\ &= \operatorname{tr}\ln\hat{G}_0^{-1} - \operatorname{tr}\left[-ie\hat{G}_0\phi + \frac{1}{2}\left(ie\hat{G}_0\phi \right)^2 + \cdots \right] \end{aligned}$$

• First order term: for convenience, set $k \equiv (\mathbf{k}, \omega_n)$, etc.

$$2\mathrm{tr}[\hat{G}_0\phi] = 2\sum_k \overbrace{\langle k|\hat{G}_0|k\rangle}^{G_0(k)} \overbrace{\frac{1}{\sqrt{L^3\beta}}\phi_{k=0}\langle k|\phi|k\rangle}^{} = \frac{2}{\sqrt{L^3\beta}}\sum_k \frac{1}{-i\omega_n + \epsilon_{\mathbf{k}} - \mu}\phi_0 = 0$$

$\phi_0 = 0$ due to neutralising background

- Second order term:

$$2 \times \frac{e^2}{2}\mathrm{tr}[\hat{G}_0\phi]^2 = e^2 \sum_{k,q} \overbrace{\langle k|\hat{G}_0|k\rangle}^{G_0(k)} \overbrace{\langle k|\phi|k+q\rangle}^{\frac{1}{\sqrt{\beta L^3}}\phi_q} \overbrace{\langle k+q|\hat{G}_0|k+q\rangle}^{G_0(k+q)} \overbrace{\langle k+q|\phi|k\rangle}^{\frac{1}{\sqrt{\beta L^3}}\phi_{-q}} = \frac{e^2}{2}\sum_q \Pi(q)\phi_{-q}\phi_q$$

where "density-density" response function,

$$\boxed{\Pi(q) = \frac{2}{\beta L^3}\sum_k \frac{1}{-i\omega_n + \epsilon_{\mathbf{k}} - \mu}\,\frac{1}{-i\omega_n - i\omega_m + \epsilon_{\mathbf{k+q}} - \mu}}$$

Combined with bare term, to leading order in e^2 (Random Phase Approximation),

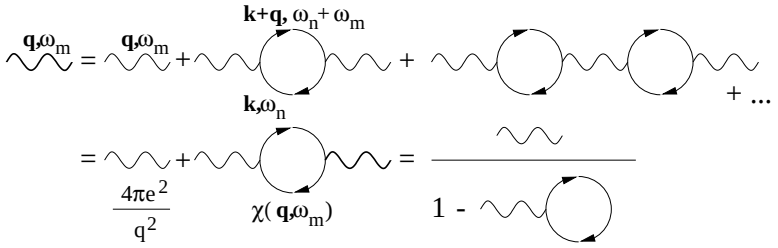
$$\mathcal{Z} = \mathcal{Z}_0 \int D\phi\, e^{-S[\phi]}, \qquad S[\phi] = \frac{1}{2}\sum_q \overbrace{\left(\frac{\mathbf{q}^2}{4\pi} - e^2\Pi(q)\right)}^{D^{-1}(q)} |\phi_q|^2 + O(e^4)$$

$\mathcal{Z}_0$ denotes partition function of non-interacting gas

▷ Physically, $D^{-1}(q)$ denotes dynamically screened Coulomb interaction

$$\boxed{D^{-1}(q) = \epsilon(q)\frac{\mathbf{q}^2}{4\pi}, \qquad \epsilon(q) = 1 - \frac{4\pi e^2}{\mathbf{q}^2}\Pi(q)}$$

where $\epsilon(q)$ is the energy and momentum dependent effective dielectric function



Diagrammatic interpretation:

$$D(q) = \frac{4\pi}{\mathbf{q}^2}\frac{1}{1 - \frac{4\pi e^2}{\mathbf{q}^2}\Pi(q)} = \frac{4\pi}{\mathbf{q}^2}\sum_{n=0}^{\infty}\left(e^2\Pi(q)\frac{4\pi}{\mathbf{q}^2}\right)^n$$

Lecture XVIII: Random Phase Approximation

▷ Previously, we have seen that the quantum partition function of the weakly interacting electron gas can be written as field integral

$$\mathcal{Z} = \mathcal{Z}_0 \int D\phi\, e^{-S[\phi]}, \qquad S[\phi] = \frac{1}{2} \sum_{q=(\omega_m,\mathbf{q})} \overbrace{\left(\frac{\mathbf{q}^2}{4\pi} - e^2 \Pi(q) \right)}^{D^{-1}(q)} |\phi_q|^2 + O(e^4)$$

where dielectric properties found to be controlled by density-density response function

$$\boxed{\Pi(q) = \frac{2}{\beta L^3} \sum_k \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} + \mu} \; \frac{1}{i\omega_n + i\omega_m - \epsilon_{\mathbf{k}+\mathbf{q}} + \mu}}$$

To understand form of $\chi(q)$, we have to digress and discuss

▷ Matsubara Summations

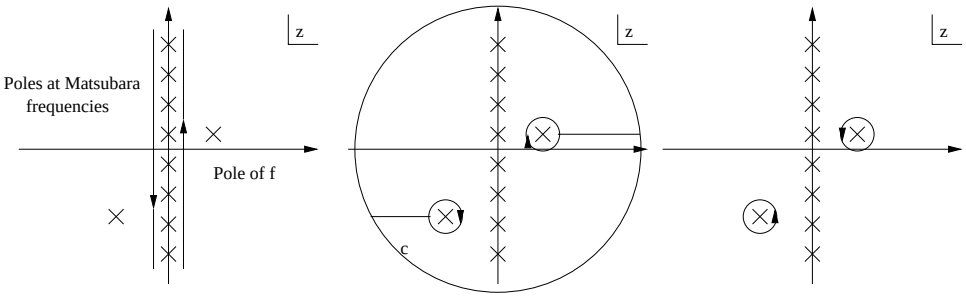
Basic idea: by introducing auxiliary function $g(z)$ that has simple poles of strength unity at $z = i\omega_n$, Cauchy's theorem implies

$$\sum_{\omega_n} f(i\omega_n) = \frac{1}{2\pi i} \oint_C dz\, g(z) f(z)$$

where contour C encloses only poles of $g(z)$

$$\text{e.g.} \quad g(z) = \begin{cases} \dfrac{\beta}{\exp(\beta z) - 1}, & \text{bosons} \\ -\dfrac{\beta}{\exp(\beta z) + 1}, & \text{fermions} \end{cases}$$

Then, moving contour to infinity



$$\sum_{\omega_n} f(i\omega_n) = \overbrace{\lim_{R\to\infty} \frac{R}{2\pi i} \int_0^{2\pi} d\theta g(Re^{i\theta}) f(Re^{i\theta})}^{\to 0} - \overbrace{\frac{1}{2\pi i} \sum_{P: f(z_P)=0} \oint dz g(z) f(z)}^{\text{if simple } \sum_P g(z_P) f(z_P)}$$

Applied to $\chi(q)$,

$$\chi(q) = -\frac{2}{\beta L^3}\sum_{\mathbf{k}}\left[\frac{g(\epsilon_{\mathbf{k}}-\mu)}{i\omega_m+\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}}}+\frac{g(\epsilon_{\mathbf{k}+\mathbf{q}}-\mu-i\frac{2\pi m}{\beta})}{-i\omega_m-\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k}+\mathbf{q}}}\right] = \frac{2}{L^3}\sum_{\mathbf{k}}\frac{n_F(\epsilon_{\mathbf{k}})-n_F(\epsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_m+\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}}},$$

where $n_{\rm F}(\epsilon) = \dfrac{1}{e^{\beta(\epsilon-\mu)}+1}$ is the Fermi distribution function
Finally, for $|\mathbf{q}| \ll k_F \equiv (2m\mu)^{1/2}$ and $k_{\rm B}T \ll \mu$, $\mathbf{k}$ summation $\rightsquigarrow$ Lindhard function

$$\chi(q) \simeq -2\nu(\mu)\left(1-\frac{\omega_m}{v_F|\mathbf{q}|}\tan^{-1}\left[\frac{v_F|\mathbf{q}|}{\omega_m}\right]\right)$$

where $\nu(\mu)$ is density of states at Fermi level

- Static Limit: For $|\omega_m| \ll k_F|\mathbf{q}|/m$, $\chi(0,\mathbf{q}) \simeq -2\nu(\mu)$, i.e.

$$D(0,\mathbf{q}) \simeq \frac{4\pi e^2}{\mathbf{q}^2}\frac{1}{1+2\frac{4\pi e^2}{\mathbf{q}^2}\nu(\mu)}$$

Fourier transformed, $\rightsquigarrow$ static screened Coulomb interaction $\dfrac{e^2}{|\mathbf{r}|}e^{-|\mathbf{r}|/\lambda_{\rm TF}}$
where $\lambda_{\rm TF} = 2\times 4\pi e^2\nu(\mu)$ — Thomas-Fermi screening length

i.e. At long time scales (low frequencies), bare Coulomb interaction is
renormalised (screened) by collective charge fluctuations

Physically, focusing a single electron, because it is negatively charged, other electrons will be repelled. As a result, a positively charged cloud of radius $\lambda_{\rm TF}$ will form balancing the negative charge of the electron. When viewed from a distance larger than $\lambda_{\rm TF}$, the electron+cloud behaves as a neutral particle.

- High Frequency Limit: For $|\omega_n| \gg k_F|\mathbf{q}|/m$, $\chi(\omega_m,\mathbf{q}) \simeq -\dfrac{\mathbf{q}^2}{m\omega_m^2}n$,
where $n = N/L^3$ is the total number density (including spin)

$$D(q) = \frac{4\pi e^2}{\mathbf{q}^2}\frac{1}{1+\frac{4\pi e^2 n}{m\omega_m^2}}$$

i.e. real time response ($i\omega_m \to \omega + i0$) singular when
$\omega_p = 4\pi e^2 n/m$ — Plasma frequency

In this case, there is a resonance which couples to the excitation mode where the positively charged background and the negatively charged electrons are moving uniformly against each other.

- Ground State Energy

$$\lim_{\beta\to\infty} \mathcal{Z} \sim e^{-\beta E_{\text{g.s.}}}.$$

In the RPA approximation, $\mathcal{Z} = \mathcal{Z}_0 \times \dfrac{\text{const.}}{\det D^{-1/2}} = \mathcal{Z}_0 \times \text{const.} \prod_{\text{q}} \text{D(q)}^{1/2}$

$$\text{i.e. } E_{\text{g.s.}} = E_{\text{g.s.}}(e=0) - \frac{1}{2\beta}\sum_{q} \ln D(q)$$

Lecture XIX: Bose-Einstein Condensation

Previously, we have seen how the functional field integral technique can be developed to explore the impact of the electronic degrees of freedom on the effective Coulomb interaction in a metal. However, our considerations did not engage any non-trivial mean-fields: the platform of the non-interacting electron system remains adiabatically connected to that of the weakly interacting system. In the following we will explore a problem in which the development of a non-trivial ground state — the Bose-Einstein condensate — is accompanied by the appearance of collective modes absent in the non-interacting system.

▷ Following our earlier considerations, we begin with a Hamiltonian describing a Bose system of size L subject to a weak short-ranged repulsive contact interaction:

$$\hat{H} = \int d^d r\, a^\dagger(\mathbf{r}) \hat{H}_0 a(\mathbf{r}) + \frac{g}{2} \int d^d r\, a^\dagger(\mathbf{r}) a^\dagger(\mathbf{r}) a(\mathbf{r}) a(\mathbf{r})$$

▷ CSPI: $\mathcal{Z} = \mathrm{tr} e^{-\beta(\hat{H}-\mu\hat{N})} = \int_{\psi(\beta)=\psi(0)} D(\bar{\psi},\psi)\, e^{-S[\bar{\psi},\psi]}$,

$$S = \int_0^\beta d\tau \int d^d r \left[\bar{\psi}(\mathbf{r},\tau)(\partial_\tau + \hat{H}_0 - \mu)\psi(\mathbf{r},\tau) + \frac{g}{2}(\bar{\psi}(\mathbf{r},\tau)\psi(\mathbf{r},\tau))^2 \right] ,$$

▷ <u>Bose-Einstein Condensation</u>

As a warm-up, consider non-interacting Bose gas with spectrum ϵ_a

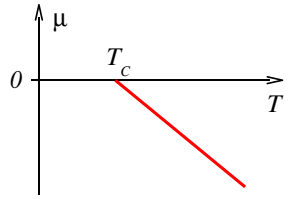
$$\mathcal{Z}_0 \equiv \mathcal{Z}\Big|_{g=0} = \int_{\text{p.b.c.}} D(\bar{\psi},\psi)\, e^{-\sum_{a\omega_n} \bar{\psi}_{a,\omega_n}(-i\omega_n+\epsilon_a-\mu)\psi_{a\omega_n}} = \text{const.} \prod_{a,\omega_n} \frac{1}{-i\omega_n+\epsilon_a-\mu}$$

where, w.l.o.g., we assume $\epsilon_a \geq 0$ and $\epsilon_0 = 0$

While stability of integral requires $\mu \leq 0$, precise value fixed by

$$N(\mu) = -\partial_\mu F = \frac{1}{\beta}\partial_\mu \ln \mathcal{Z}_0 = -\frac{1}{\beta}\sum_{a,\omega_n} \frac{1}{i\omega_n - \epsilon_a + \mu} = \sum_a n_{\mathrm{B}}(\epsilon_a) ,$$

where, using Matsubara summation, $n_{\mathrm{B}}(\epsilon) = \dfrac{1}{e^{\beta(\epsilon-\mu)}-1}$ (Bose-Einstein distribution)



As T reduced, μ increased until, at $T = T_{\mathrm{BEC}}$, $\mu = 0$. For $T < T_{\mathrm{BEC}}$, μ remains zero and a macroscopic number of particles $N - N_1$ condense into ground state: <u>Bose-Einstein condensation</u>

$$\text{i.e. for } T < T_{\mathrm{BEC}}, \qquad \sum_{a>0} n_{\mathrm{B}}(\epsilon_a)\Big|_{\mu=0} \equiv N_1 < N$$

▷ How can this phenomenon be incorporated into the path integral?

Although condensate characterised by ground state component $\psi_0(\tau)$
for $T < T_{\rm BEC}$, fluctuations are unbound ($\mu = 0 = \epsilon_0$ and action for $\psi_{0,0}$ vanishes!)

Here we must treat field $\psi_0(\tau)$ as a (time-independent)
Lagrange multiplier to be used to fix the number of particles below $T_{\rm BEC}$:

$$S_0|_{\mu=0^-} \simeq -\beta\bar{\psi}_0\mu\psi_0 + \sum_{a\neq 0,\omega_n} \bar{\psi}_{a\omega_n}\left(-i\omega_n + \epsilon_a - \mu\right)\psi_{a\omega_n}$$

$$\text{i.e. } N = -\partial_\mu F|_{\mu=0^-} = \frac{1}{\beta}\partial_\mu \ln \mathcal{Z}_0|_{\mu=0^-} = \bar{\psi}_0\psi_0 - \frac{1}{\beta}\sum_{a\neq 0,\omega_n}\frac{1}{i\omega_n - \epsilon_a} = \bar{\psi}_0\psi_0 + N_1$$

i.e. $\bar{\psi}_0\psi_0 = N_0$ translates to number of particles in condensate

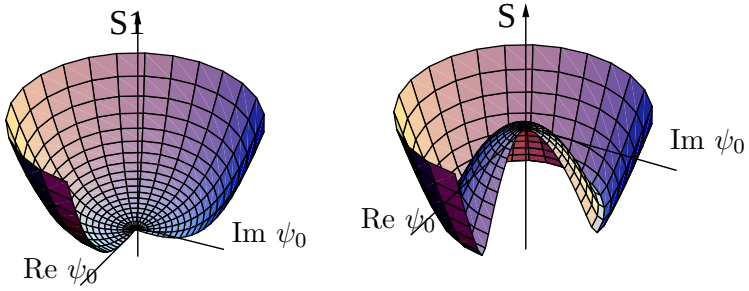
▷ <u>Weakly Interacting Bose Gas</u>

As in electron gas Presence of interaction prevents exact evaluation of field integral
therefore, turn to saddle-point + fluctuations analysis

▷ <u>Landau theory</u>

In saddle-point (mean-field) approximation dominant contribution to $\mathcal{Z} = \int D(\bar{\psi},\psi)e^{-S}$
controlled by $\psi_0(\omega_n = 0)$ (i.e. time-independent) sector of theory

$$\boxed{\frac{1}{\beta}S[\bar{\psi}_0,\psi_0] = -\mu\bar{\psi}_0\psi_0 + \frac{g}{2L^d}(\bar{\psi}_0\psi_0)^2}$$



Minimum action obtained from saddle-point equation: $\psi_0(-\mu + \frac{g}{L^d}\bar{\psi}_0\psi_0) = 0$

▷ For $\mu < 0$ (i.e. above the condensation threshold of the non-interacting system),
s.p.e. exhibits only trivial solution $\psi_0 = 0$ — no stable condensate

▷ Below condensation threshold (i.e. for $\mu \geq 0$), equation solved by any
configuration with $|\psi_0| = \gamma \equiv \sqrt{\mu L^d/g}$

N.B. $\bar{\psi}_0\psi_0 \propto L^d$, reflecting the macroscopic population of the ground state

▷ The equation couples only to the modulus of ψ_0, i.e. the solution of the stationary phase equation is "continuously degenerate": Each configuration $\psi_0 = \gamma \exp(i\phi), \phi \in [0, 2\pi]$ is a solution. One ground state chosen $\rightsquigarrow$ spontaneous symmetry breaking.

Self-consistent calculation of $\mu = \mu(N)$ demands consideration
of low-energy fluctuations around the mean-field solution

By taking into account such fluctuations, we will be also able
to address the phenomenon of superfluidity

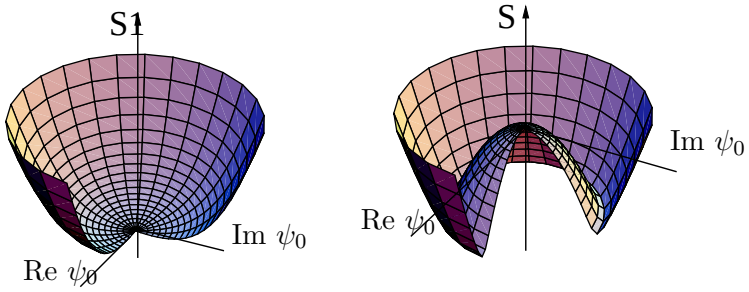
Lecture XX: Superfluidity

Previously, we have seen that, when treated in a mean-field or saddle-point approximation, the field theory of the weakly interacting Bose gas shows a transition to a Bose-Einstein condensed phase when $\mu = 0$ where the order parameter, the complex condensate wave-function ψ_0 acquires a non-zero expectation value, $|\psi_0| = \gamma \equiv \sqrt{\mu L^d/g}$. The spontaneous breaking of the continuous symmetry associated with the phase of the order parameter is accompanied by the appearance of massless collective phase fluctuations. In the following, we will explore the properties of these fluctuations and their role in the phenomenon of superfluidity.

▷ Starting with model action for the Bose system, ($\hbar = 1$)

$$S[\bar{\psi},\psi] = \int_0^\beta d\tau \int d^d r \left[\bar{\psi}(\mathbf{r},\tau)\left(\partial_\tau - \frac{\partial^2}{2m} - \mu\right)\psi(\mathbf{r},\tau) + \frac{g}{2}(\bar{\psi}(\mathbf{r},\tau)\psi(\mathbf{r},\tau))^2\right]$$

a saddle-point analysis of the action revealed that, for $\mu > 0$, the field ψ acquires a constant non-zero expectation value: $\bar{\psi}_0 = \psi_0 = (\mu L^d/g)^{1/2} \equiv \gamma$



In the following, we will explore the effect of fluctuations around the mean-field

To do so, it is convenient to effect the reparameterisation $\psi(\mathbf{r},\tau) = [\rho(\mathbf{r},\tau)]^{1/2} e^{i\phi(\mathbf{r},\tau)}$

$$\frac{1}{2}\int_0^\beta d\tau \partial_\tau(\rho^{1/2}\rho^{1/2}) = -\frac{\rho}{2}\Big|_0^\beta = 0$$

Using 1. $\displaystyle\int_0^\beta d\tau \bar{\psi}\partial_\tau\psi = \overbrace{\int_0^\beta d\tau \rho^{1/2}\partial_\tau\rho^{1/2}} + \int_0^\beta d\tau i\rho\partial_\tau\phi$

2. $\partial(\rho^{1/2}e^{i\phi}) = \left(\frac{1}{2\rho^{1/2}}\partial\rho + i\rho^{1/2}\partial\phi\right)e^{i\phi}$

3. $\displaystyle\int_0^\beta d\tau \bar{\psi}\partial^2\psi = -\int_0^\beta d\tau \partial\bar{\psi}\cdot\partial\psi = -\int_0^\beta \left(\frac{1}{4\rho}(\partial\rho)^2 + \rho(\partial\phi)^2\right)$

the action takes the form

$$S[\rho,\phi] = \int_0^\beta d\tau \int d^d r \left\{ i\rho\partial_\tau\phi + \frac{1}{2m}\left[\frac{1}{4\rho}(\partial\rho)^2 + \rho(\partial\phi)^2\right] - \mu\rho + \frac{g\rho^2}{2}\right\}$$

Then, discarding gradient terms involving massive fluctuations $\delta\rho$,

an expansion in $\delta\rho \equiv \rho - \rho_0$ at $\mu = \mu_{\rm BEC} = 0$

$$S[\delta\rho,\phi] \simeq S_0[\rho_0] + \int_0^\beta d\tau \int d^d r \left[i\delta\rho\partial_\tau\phi + \frac{g\delta\rho^2}{2} + \frac{\rho_0}{2m}(\partial\phi)^2 \right]$$

- First term has canonical structure 'momentum $\times\, \partial_\tau$ (coordinate)'

  cf. canonically conjugate pair

- Second term records energy cost of "massive" fluctuations from

  Mexican hat potential minimum

- Third term measures energy cost of spatially varying massless phase flucutations:

  i.e. ϕ is a Goldstone mode

Gaussian integration over $\delta\rho$:

$$\frac{g}{2}\left(\delta\rho + \frac{i}{g}\partial_\tau\phi\right)^2 + \frac{(\partial_\tau\phi)^2}{2g}$$

$$\int D(\delta\rho) \exp\Big[-\int_0^\beta d\tau \int d^d r \overbrace{\left(i\delta\rho\partial_\tau\phi + \frac{g\delta\rho^2}{2} \right)} \Big] = \text{const.} \times \exp\left[-\int_0^\beta d\tau \int d^d r \frac{(\partial_\tau\phi)^2}{2g} \right]$$

$\rightsquigarrow$ effective low energy action

$$S[\phi] \simeq S_0 + \frac{1}{2}\int_0^\beta d\tau \int d^d r \left[\frac{1}{g}(\partial_\tau\phi)^2 + \frac{\rho_0}{m}(\partial\phi)^2 \right] .$$

cf. Lagrangian formulation of harmonic medium (or massless Klein-Gordon field)

$$S = \int dt \int d^d r \left[\frac{m}{2}\dot{\phi}^2 - \frac{1}{2}k_s a^2 (\partial\phi)^2 \right] = \int dx\, \partial^\mu\phi\partial_\mu\phi$$

i.e. low-energy excitations involve collective phase fluctuations with a spectrum $\omega_{\mathbf{k}} = \dfrac{g\rho_0}{m}|\mathbf{k}|$

▷ PHYSICAL RAMIFICATIONS: consider quantum mechanical current density operator

$$\hat{\mathbf{j}}(\mathbf{r},\tau) = \frac{1}{2}\left[a^\dagger(\mathbf{r},\tau)\frac{\hat{\mathbf{p}}}{m}a(\mathbf{r},\tau) - \left(\frac{\hat{\mathbf{p}}}{m}a^\dagger(\mathbf{r},\tau)\right) a(\mathbf{r},\tau) \right]$$
$$\stackrel{\text{fun. int}}{\longrightarrow} \frac{i}{2m}\left[(\partial\bar{\psi}(\mathbf{r},\tau))\psi(\mathbf{r},\tau) - \bar{\psi}(\mathbf{r},\tau)\partial\psi(\mathbf{r},\tau) \right] \simeq \frac{\rho_0}{m}\partial\phi(\mathbf{r},\tau)$$

i.e. $\partial\phi$ is measure of (super)current flow

Variation of action $S[\delta,\phi] \rightsquigarrow$

$$i\partial_\tau\phi = -g\delta\rho, \qquad i\partial_\tau\delta\rho = \frac{\rho_0}{m}\partial^2\phi = \partial\cdot\mathbf{j}$$

- First equation: system adjusts to spatial fluctuations of density

  by dynamical phase fluctuation

- Second equation $\rightsquigarrow$ continuity equation (conservation of mass)

Crucially, stationary equations possess steady state solution with non-vanishing current flow: setting $\partial_\tau \phi = \partial_\tau \delta\rho = 0$, obtain $\delta\rho = 0$ and $\partial \cdot \mathbf{j} = 0$

i.e. for $T < T_{\rm BEC}$, a configuration with a uniform density profile can support a steady state divergenceless (super)flow

Notice that a 'mass term' in the phase ϕ action would spoil this property, i.e. the phenomenon of superflow is intimately linked to the Goldstone mode

▷ Steady state current flow in normal environments is prevented by the mechanism of energy dissipation, i.e. particles scatter off imperfections inside the system and thereby converting part of their energy into the creation of elementary excitations

How can dissipative loss of energy be avoided?

Trivially, no energy can be exchanged if there are no elementary excitations to create

In reality, this means that the excitations of the system should be energetically inaccessible (k.e. of carriers too small to create excitations)

But this is not the case here! there is no energy gap ($\omega_{\mathbf{k}} \propto |\mathbf{k}|$)

However, there is an ingenuous argument due to Landau (see notes) showing that a linear excitation spectrum can stabilize dissipationless transport

Lecture XXI: Cooper instability

In the final section of the course, we will explore a pairing instability of the electron gas which leads to condensate formation and the phenomenon of superconductivity.

▷ History:

- 1911 discovery of superconductivity (Onnes)
- 1951 "isotope effect" — clue to (conventional) mechanism
- 1956 Development of (correct) phenomenology (Ginzburg-Landau)
- 1957 BCS theory of conventional superconductivity (Bardeen-Cooper-Schrieffer)
- 1976 Discovery of unconventional superconductivity in heavy fermions (Steglich)
- 1986 Discovery of high temperature superconductivity in cuprates (Bednorz-Müller)
- ???? awaiting theory?

▷ (Conventional) mechanism: exchange of phonons can induce (space-nonlocal) attractive pairwise interaction between electrons

$$\hat{H}' = \hat{H}_0 - |M|^2 \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{\hbar\omega_{\mathbf{q}}}{\hbar^2\omega_{\mathbf{q}}^2 - (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}})^2} c^\dagger_{\mathbf{k}-\mathbf{q}\sigma} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}$$

Physically electrons can lower their energy by sharing lattice polarisation of another

By exploiting interaction, electron pairs can condense into macroscopic phase coherent state with energy gap to quasi-particle excitations

To understand why, let us consider the argument marshalled by Cooper which lead to the development of a consistent many-body theory.

▷ <u>Cooper instability</u>

Consider two electrons propagating above a filled Fermi sea:
Is a weak pairwise interaction $V(\mathbf{r}_1 - \mathbf{r}_2)$ sufficient to create a bound state?

Consider variational state

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \overbrace{\frac{1}{\sqrt{2}}(|\uparrow_1\rangle \otimes |\downarrow_2\rangle - |\uparrow_2\rangle \otimes |\downarrow_1\rangle)}^{\text{spin singlet}} \overbrace{\sum_{|\mathbf{k}|\geq k_F} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}}^{\text{spatial symm. } g_{\mathbf{k}} = g_{-\mathbf{k}}}$$

Applied to Schrödinger equation: $\hat{H}\psi = E\psi$

$$\sum_{\mathbf{k}} g_{\mathbf{k}} \left[2\epsilon_{\mathbf{k}} + V(\mathbf{r}_1 - \mathbf{r}_2)\right] e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} = E \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}$$

Fourier transforming equation: $\times L^{-d}\int d(\mathbf{r}_1-\mathbf{r}_2)e^{-i\mathbf{k}'\cdot(\mathbf{r}_1-\mathbf{r}_2)}$

$$\sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'}g_{\mathbf{k}'} = (E-2\epsilon_{\mathbf{k}})g_{\mathbf{k}}, \qquad V_{\mathbf{k}\mathbf{k}'} = \frac{1}{L^d}\int d\mathbf{r}\, V(\mathbf{r})e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}$$

If we assume $V_{\mathbf{k}-\mathbf{k}'} = \begin{cases} -\frac{V}{L^d} & \{|\epsilon_{\mathbf{k}}-\epsilon_F|, |\epsilon_{\mathbf{k}'}-\epsilon_F|\} < \omega_D \\ 0 & \text{otherwise} \end{cases}$

$$-\frac{V}{L^d}\sum_{\mathbf{k}'} g_{\mathbf{k}'} = (E-2\epsilon_{\mathbf{k}})g_{\mathbf{k}} \mapsto -\frac{V}{L^d}\sum_{\mathbf{k}}\frac{1}{E-2\epsilon_{\mathbf{k}}}\sum_{\mathbf{k}'} g_{\mathbf{k}'} = \sum_{\mathbf{k}} g_{\mathbf{k}} \mapsto -\frac{V}{L^d}\sum_{\mathbf{k}}\frac{1}{E-2\epsilon_{\mathbf{k}}} = 1$$

Using $\frac{1}{L^d}\sum_{\mathbf{k}} = \int\frac{d^dk}{(2\pi)^d} = \int\nu(\epsilon)\,d\epsilon \sim \nu(\epsilon_F)\int d\epsilon$, where $\nu(\epsilon) = \frac{1}{|\partial_{\mathbf{k}}\epsilon_{\mathbf{k}}|}$ is DoS

$$\frac{V}{L^d}\sum_{\mathbf{k}}\frac{1}{2\epsilon_{\mathbf{k}}-E} \simeq \nu(\epsilon_F)V\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{d\epsilon}{2\epsilon-E} = \frac{\nu(\epsilon_F)V}{2}\ln\left(\frac{2\epsilon_F+2\omega_D-E}{2\epsilon_F-E}\right) = 1$$

In limit of weak coupling, i.e. $\nu(\epsilon_F)V \ll 1$

$$E \simeq 2\epsilon_F - 2\omega_D e^{-\frac{2}{\nu(\epsilon_F)V}}$$

- i.e. pair forms a bound state (no matter how small interaction!)
- energy of bound state is non-perturbative in $\nu(\epsilon_F)V$

▷ Radius of pair wavefunction: $g(\mathbf{r}) = \sum_{\mathbf{k}} g_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$, $g_{\mathbf{k}} = \frac{1}{2\epsilon_{\mathbf{k}}-E}\times$ const., $\partial_{\mathbf{k}} = \frac{\partial\epsilon_{\mathbf{k}}}{\partial\mathbf{k}}\frac{\partial}{\partial\epsilon}$

$$\langle\mathbf{r}^2\rangle = \frac{\int d^dr\ \mathbf{r}^2|g(\mathbf{r})|^2}{\int d^dr|g(\mathbf{r})|^2} = \frac{\sum_{\mathbf{k}}|\partial_{\mathbf{k}}g_{\mathbf{k}}|^2}{\sum_{\mathbf{k}}|g_{\mathbf{k}}|^2} \simeq \frac{v_F^2\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{4d\epsilon}{(2\epsilon-E)^4}}{\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{d\epsilon}{(2\epsilon-E)^2}} = \frac{4}{3}\frac{v_F^2}{(2\epsilon_F-E)^2}$$

if binding energy $2\epsilon_F - E \sim k_{\rm B}T_c$, $T_c \sim 10$K, $v_F \sim 10^8$cm/s, $\xi_0 = \langle\mathbf{r}^2\rangle^{1/2} \sim 10^4\mathring{A}$,
i.e. other electrons must be important

▷ BCS WAVEFUNCTION

Two electrons in a paired state has wavefunction

$$\phi(\mathbf{r}_1-\mathbf{r}_2) = (|\uparrow_1\rangle\otimes|\downarrow_2\rangle - |\downarrow_1\rangle\otimes|\uparrow_2\rangle)g(\mathbf{r}_1-\mathbf{r}_2)$$

with zero centre of mass momentum

Drawing analogy with Bose condensate, let us examine variational state

$$\psi(\mathbf{r}_1\cdots\mathbf{r}_{2N}) = \mathcal{N}\prod_{n=1}^{N}\phi(\mathbf{r}_{2n-1}-\mathbf{r}_{2n})$$

Is state compatible with Pauli principle? Using $g(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}$
or, in Fourier representation

$$\int \frac{d^d r_1}{L^d} e^{-i\mathbf{k}_1\cdot\mathbf{r}_1} \int \frac{d^d r_2}{L^d} e^{-i\mathbf{k}_2\cdot\mathbf{r}_2} g(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} g_{\mathbf{k}} \delta_{\mathbf{k}_1,\mathbf{k}} \delta_{\mathbf{k}_2,-\mathbf{k}}$$

or in second quantised form,

$$\text{FT}\left[g(\mathbf{r}_1 - \mathbf{r}_2) c^\dagger_\uparrow(\mathbf{r}_1) c^\dagger_\downarrow(\mathbf{r}_2) |\Omega\rangle \right] = \sum_{\mathbf{k}} g_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} |\Omega\rangle$$

Then, of the terms in the expansion of

$$|\psi\rangle = \prod_{n=1}^{N} \left[\sum_{\mathbf{k}_n} g_{\mathbf{k}_n} c^\dagger_{\mathbf{k}_n\uparrow} c^\dagger_{-\mathbf{k}_n\downarrow} \right] |\Omega\rangle$$

those with all $\mathbf{k}_n$s different survive

Generally, more convenient to work in grand canonical ensemble
where one allows for (small) fluctuations in the total particle density

$$|\psi\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}) |\Omega\rangle \;\; \overbrace{\sim \exp\left[\sum_{\mathbf{k}} g_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right] |\Omega\rangle}^{\text{cf. coherent state}}$$

i.e. statistical independence of pair occupation

In non-interacting electron gas $v_{\mathbf{k}} = \begin{cases} 1 & |\mathbf{k}| < k_F \\ 0 & |\mathbf{k}| > k_F \end{cases}$

In interacting system, to determine the variational parameters $v_{\mathbf{k}}$,
one can use a variational principle, i.e. to minimise

$$\langle \psi | \hat{H} - \epsilon_F \hat{N} | \psi \rangle$$

▷ BCS Hamiltonian

However, since we are interested in both the ground state energy, and the spectrum of quasi-particle excitations, we will follow a different route and explore a simplified model Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V \sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$$

Lecture XXII: BCS Superconductivity

▷ Recall: We have seen that phonon exchange $\rightsquigarrow$ a pairing interaction which renders a single pair of electrons unstable towards the formation of a bound state (Cooper)

Motivated by this consideration, we have proposed a many-body generalisation of the pair state in the form of the variational BCS state

$$|\psi\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|\Omega\rangle$$

and within which one may show that the "anomalous average" $\bar{b}_{\mathbf{k}} = \langle\psi|c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}|\psi\rangle$ acquires a non-zero expectation

In principle, we could now proceed with the Ansatz for $|\psi\rangle$ and employ a variational analysis. However, instead, we will make use of this Ansatz to develop an approximation scheme to expand the second quantised BCS Hamiltonian. Indeed, such an approach will lead to the same phenomenology.

Since we expect quantum fluctuations in $\bar{b}_{\mathbf{k}}$ to be small, we may set

$$c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} = \bar{b}_{\mathbf{k}} + \overbrace{c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} - \bar{b}_{\mathbf{k}}}^{\text{small}}$$

(cf. our approach to BEC where $a_0^\dagger$ was replaced by a C-number) so that

$$\begin{aligned}
\hat{H} - \mu\hat{N} &= \sum_{\mathbf{k}\sigma} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V \sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \qquad \zeta_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu \\
&\simeq \sum_{\mathbf{k}\sigma} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V \sum_{\mathbf{k}\mathbf{k}'} \left(\bar{b}_{\mathbf{k}} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} + b_{\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - \bar{b}_{\mathbf{k}} b_{\mathbf{k}'} \right)
\end{aligned}$$

Then, if we set $V\sum_{\mathbf{k}} b_{\mathbf{k}} \equiv \Delta$, we obtain Bogoliubov-de Gennes or Gor'kov Hamiltonian

$$\begin{aligned}
\hat{H} - \mu\hat{N} &= \sum_{\mathbf{k}} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left(\bar{\Delta} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} + \Delta c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right) + \frac{|\Delta|^2}{V} \\
&= \sum_{\mathbf{k}} \begin{pmatrix} c^\dagger_{\mathbf{k}\uparrow} & c_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \zeta_{\mathbf{k}} & -\Delta \\ -\bar{\Delta} & -\zeta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} + \frac{|\Delta|^2}{V}
\end{aligned}$$

For simplicity, let us for now assume that Δ is real

Bilinear in fermion operators, $\hat{H} - \mu\hat{N}$ is diagonalised by canonical transformation

$$\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} = \overbrace{\begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix}}^{\mathrm{O}^T} \begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}$$

where anticommutation relation requires $O^T O = \mathbf{1}$,
i.e. $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ (orthogonal transformations)

Substituting, one finds that the Hamiltonian diagonalised if

$$2\zeta_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \Delta(v_k^2 - u_{\mathbf{k}}^2) = 0$$

i.e. setting $u_k = \sin\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \cos\theta_{\mathbf{k}}$,

$$\tan 2\theta_{\mathbf{k}} = -\frac{\Delta}{\zeta}, \qquad \sin 2\theta_{\mathbf{k}} = \frac{\Delta}{\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}}, \qquad \cos 2\theta_{\mathbf{k}} = -\frac{\zeta_{\mathbf{k}}}{\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}}$$

(N.B. for complex $\Delta = |\Delta| e^{i\phi}$, $v_{\mathbf{k}} = e^{i\phi}\cos\theta_{\mathbf{k}}$)

As a result

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}} (\zeta_{\mathbf{k}} - (\zeta_{\mathbf{k}}^2 + \Delta^2)^{1/2}) - \frac{\Delta^2}{V} + \sum_{\mathbf{k}\sigma} (\zeta_{\mathbf{k}}^2 + \Delta^2)^{1/2} \gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}\sigma}$$

Quasi-particle excitations, created by $\gamma_{\mathbf{k}\sigma}^\dagger$, have minimum energy Δ

Energy gap $\rightsquigarrow$ rigidity of ground state

Ground state wavefunction identified as vacuum state of algebra $\{\gamma_{\mathbf{k}\sigma}, \gamma_{\mathbf{k}\sigma}^\dagger\}$,

i.e state which is annihilated by all the quasi-particle operators $\gamma_{\mathbf{k}\sigma}$.

Condition met uniquely by the state

$$|\psi\rangle \equiv \prod_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}\gamma_{\mathbf{k}\uparrow}|\Omega\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} - v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger)(u_{\mathbf{k}} c_{\mathbf{k}\uparrow} + v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger)|\Omega\rangle$$
$$= \prod_{\mathbf{k}} (v_{\mathbf{k}})(u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow}^\dagger - v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|\Omega\rangle = \text{const.} \times \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger\right)|\Omega\rangle$$

cf. variational analysis — in fact, const. = 1

Note that phase of Δ is arbitrary,

i.e. ground state is continuously degenerate (cf. BEC)

▷ Self-consistency condition: <u>BCS gap equation</u>

$$\Delta = V\sum_{\mathbf{k}} b_{\mathbf{k}} = V\sum_{\mathbf{k}} \langle\psi| c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger |\psi\rangle = V\sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} = \frac{V}{2}\sum_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} = \frac{V}{2}\sum_{\mathbf{k}} \frac{\Delta}{\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}}$$

$$\text{i.e.} \quad 1 = \frac{V}{2}\sum_{\mathbf{k}} \frac{1}{\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}} = \frac{VL^d\nu(\epsilon_F)}{2}\int_{-\omega_D}^{\omega_D} d\zeta \frac{1}{\sqrt{\zeta^2 + \Delta^2}}$$

if $\omega_D \gg \Delta$, $\Delta \simeq 2\omega_D e^{-\frac{1}{\nu(\epsilon_F)VL^d}}$

<u>Ground state:</u> In limit $\Delta \to 0$, $v_{\mathbf{k}}^2 \mapsto \theta(\epsilon_F - \epsilon_{\mathbf{k}})$, and the ground state collapses to the filled Fermi sea with chemical potential ϵ_F

As Δ becomes non-zero, states in the vicinity of the Fermi surface rearrange into a condensate of paired states

Excitations: Spectrum of quasi-particle excitations $\sqrt{\zeta_{\mathbf{k}}^2 + \Delta^2}$ shows rigid energy gap Δ. An excitation can be either the creation of a quasi-particle at positive energy or the elimination of a quasi-particle (the creation of a quasi-hole) at negative energy. In the ground state, all negative-energy quasi-particle states are filled.

Density of quasi-particle excitations near Fermi surface

$$\rho(\epsilon) = \frac{1}{L^d}\sum_{\mathbf{k}\sigma}\delta(\epsilon - \sqrt{\zeta_{\mathbf{k}} + \Delta^2}) = \int d\zeta \underbrace{\frac{1}{L^d}\sum_{\mathbf{k}\sigma}\delta(\zeta - \zeta_{\mathbf{k}})}_{\nu(\zeta)}\delta(\epsilon - \sqrt{\zeta + \Delta^2})$$

$$\approx \nu(\epsilon_F)\sum_{s=\pm 1}\int_0^\infty d\zeta \frac{\delta\left(\zeta - s[\epsilon^2 - \Delta^2]^{1/2}\right)}{\left|\frac{\partial[\zeta^2+\Delta^2]^{1/2}}{\partial\zeta}\right|} = 2\nu(\epsilon_F)\Theta(\epsilon - \Delta)\frac{\epsilon}{(\epsilon^2 - \Delta^2)^{1/2}},$$

Spectral weight transferred from Fermi surface to interval $[\Delta, \infty]$

Lecture XXIII: Field Theory of Superconductivity

Following our discussion of the field theory of BEC and superfluidity in the weakly interacting Bose gas, we turn now to condensation phenomena in Fermi systems

▷ Starting point is BCS Hamiltonian for local pairing interaction: $g \equiv \frac{V}{L^d}$

$$\hat{H} = \int d^d r \left[\sum_\sigma c_\sigma^\dagger(\mathbf{r}) \frac{\hat{\mathbf{p}}^2}{2m} c_\sigma(\mathbf{r}) - g\, c_\uparrow^\dagger(\mathbf{r}) c_\downarrow^\dagger(\mathbf{r}) c_\downarrow(\mathbf{r}) c_\uparrow(\mathbf{r}) \right]$$

▷ Quantum partition function: $\mathcal{Z} = \mathrm{tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$

$$\mathcal{Z} = \int_{\psi(\beta)=-\psi(0)} D(\bar{\psi},\psi) \exp\Big\{ - \overbrace{\int_0^\beta d\tau d^d r}^{x\equiv(\tau,\mathbf{r}) \quad \int dx} \Big[\sum_\sigma \bar{\psi}_\sigma \overbrace{\left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu \right)}^{[\hat{G}_0^{(\mathrm{p})}]^{-1}} \psi_\sigma - g \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \Big] \Big\}$$

where $\psi_\sigma(\mathbf{r},\tau)$ denote Grassmann (anticommuting) fields

Analysis of interacting QFT?

- Perturbative expansion in g?
  Transition to condensate non-perturbative in g
- "Mean-field" analysis:
  condensation of pair wavefunction signalled by "anomalous average" $\langle c_\uparrow^\dagger c_\downarrow^\dagger \rangle$

▷ Hubbard-Stratonovich" decoupling: introducing complex commuting field $\Delta(\mathbf{r},\tau)$

$$e^{g\int dx\, \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow} = \int D(\bar{\Delta},\Delta) \exp\Big\{ - \int dx \overbrace{\Big[\frac{1}{g}|\Delta(\mathbf{r},\tau)|^2 + (\bar{\Delta}\psi_\downarrow\psi_\uparrow + \Delta\bar{\psi}_\uparrow\bar{\psi}_\downarrow) \Big]}^{\frac{1}{g}(\bar{\Delta}+g\bar{\psi}_\uparrow\bar{\psi}_\downarrow)(\Delta+g\psi_\downarrow\psi_\uparrow)-g\bar{\psi}_\uparrow\bar{\psi}_\downarrow\psi_\downarrow\psi_\uparrow} \Big\}$$

$$\mathcal{Z} = \int D(\bar{\psi},\psi) \int D(\bar{\Delta},\Delta) e^{-\int dx \frac{|\Delta|^2}{g}} \exp\Big[- \int dx \overbrace{\begin{pmatrix} \bar{\psi}_\uparrow & \psi_\downarrow \end{pmatrix}}^{\text{Nambu spinor}} \overbrace{\begin{pmatrix} [\hat{G}_0^{(\mathrm{p})}]^{-1} & \Delta \\ \bar{\Delta} & [\hat{G}_0^{(\mathrm{h})}]^{-1} \end{pmatrix}}^{\text{Gor'kov Ham. } \hat{\mathcal{G}}^{-1}} \begin{pmatrix} \psi_\uparrow \\ \bar{\psi}_\downarrow \end{pmatrix} \Big]$$

'free particle/hole' Hamiltonian: $[\hat{G}_0^{(\mathrm{p/h})}]^{-1} = \partial_\tau {}^+\!/_-(\frac{\hat{\mathbf{p}}^2}{2m} - \mu)$

N.B. $\int dx\, \bar{\psi}_\downarrow \partial_\tau \psi_\downarrow = -\int dx\, (\partial_\tau \bar{\psi}_\downarrow)\psi_\downarrow = \int dx\, \psi_\downarrow \partial_\tau \bar{\psi}_\downarrow$

Using Gaussian field integral: $\int D(\bar{\psi},\psi) \exp[-\int \bar{\psi}\hat{A}\psi] = \det \hat{A} = \exp[\ln\det \hat{A}]$

$$\mathcal{Z} = \int D(\bar{\Delta},\Delta) \exp\left[- \int dx \frac{1}{g}|\Delta|^2 + \ln\det \hat{\mathcal{G}}^{-1}[\Delta] \right]$$

i.e. $\mathcal{Z}$ expressed as functional field integral over single complex scalar field $\Delta(x)$

▷ To proceed, we must invoke some approximation:

- Mean-field theory: far below transition ($T \ll T_c$, $\beta \gg \beta_c$) fluctuations small
  $\rightsquigarrow$ saddle-point approximation in Δ constant — Gap equation
- Ginzburg-Landau theory: since transition is continuous, close to T_c,
  we may develop perturbative expansion in (small) Δ

$$\text{Noting}: \qquad \hat{\mathcal{G}}^{-1} = \hat{\mathcal{G}}_0^{-1}\left[1 + \hat{\mathcal{G}}_0 \begin{pmatrix} 0 & \Delta \\ \bar{\Delta} & 0 \end{pmatrix}\right], \qquad \hat{\mathcal{G}}_0 \equiv \hat{\mathcal{G}}(\Delta = 0)$$

$$\ln\det\hat{\mathcal{G}}^{-1} = \mathrm{tr}\ln\hat{\mathcal{G}}^{-1} = \mathrm{tr}\ln\hat{\mathcal{G}}_0^{-1} - \frac{1}{2}\mathrm{tr}\left[\hat{\mathcal{G}}_0 \begin{pmatrix} 0 & \Delta \\ \bar{\Delta} & 0 \end{pmatrix}\right]^2 + \cdots$$

N.B. $\ln(1+z) = -\sum_{n=1}^{\infty}(-z)^n/n$

- Zeroth order term $\rightsquigarrow$ 'free particle' contribution, viz. $\mathcal{Z}_0 = \det\hat{\mathcal{G}}_0^{-1}$

$$\text{Using} \quad \text{id.} = \sum_{k\equiv\mathbf{k},\omega_n} |k\rangle\langle k|, \qquad \Delta_k = \frac{1}{\sqrt{\beta L^d}}\int dx \quad \overbrace{e^{ik\cdot x}}^{e^{i\omega_n\tau - i\mathbf{k}\cdot\mathbf{r}}} \quad \Delta(x)$$

- Second order term

$$\mathrm{tr}\ \hat{G}_0^{(\mathrm{p})}\Delta\hat{G}_0^{(\mathrm{h})}\bar{\Delta} \quad = \quad \sum_{kk'} G_0^{(\mathrm{p})}(k) \overbrace{\langle k|\Delta|k'\rangle}^{\Delta_{k'-k}/\sqrt{\beta L^d}} G_0^{(\mathrm{h})}(k')\langle k'|\bar{\Delta}|k\rangle$$

$$\overset{q=k'-k}{=} \sum_q \Delta_q\bar{\Delta}_{-q} \overbrace{\frac{1}{\beta L^d}\sum_k G_0^{(\mathrm{p})}(k)G_0^{(\mathrm{h})}(k+q)}^{\text{pairing susceptibility } \Pi(q)}$$

Combined with bare term, one obtains

$$\mathcal{Z} = \int D[\bar{\Delta},\Delta]e^{-S[\bar{\Delta},\Delta]}, \qquad S = \sum_{\omega_n,\mathbf{q}}\left[\frac{1}{g} + \Pi(\omega_n,\mathbf{q})\right]|\Delta_{\omega_n,\mathbf{q}}|^2 + O(\Delta^4)$$

In principle, one can evaluate $\Pi(\mathbf{q},\omega_n)$ explicitly;
however we can proceed more simply by considering...

▷ 'Gradient expansion': $\Pi(\mathbf{q},\omega_n) = \Pi(0,0) + \frac{\mathbf{q}^2}{2}\partial^2_{|\mathbf{q}|}\Pi(0,0) + O(i\omega_n,\mathbf{q}^4)$
$\rightsquigarrow$ <u>Ginzburg-Landau theory</u>

$$S[\Delta] = \beta\int d^dr\left[\frac{t}{2}|\Delta|^2 + \frac{K}{2}|\partial\Delta|^2 + u|\Delta|^4 + \cdots\right]$$

$\frac{t}{2} = \frac{1}{g} + \Pi(0,0)$, $K = \partial^2_{|\mathbf{q}|}\Pi(0,0) > 0$ and $u > 0$

Note structural similarity to weakly interacting Bose gas

▷ LANDAU THEORY: If we assume that dominant contribution to $\mathcal{Z} = e^{-\beta F}$ arises from minumum action, i.e. spatially homogeneous Δ that minimises

$$\frac{S[\Delta]}{\beta L^d} = \frac{t}{2}|\Delta|^2 + u|\Delta|^4$$

$$\text{i.e.} \quad |\Delta|\left(t + 4u|\Delta|^2\right) = 0, \qquad |\Delta| = \begin{cases} 0 & t > 0 \\ \sqrt{t/4u} & t < 0 \end{cases}$$

i.e. for $t < 0$, spontaneous breaking of continuous U(1) symmetry associated with phase $\rightsquigarrow$ gapless fluctuations — Goldstone modes

▷ TRANSITION TEMPERATURE: Using identity $\frac{1}{L^d}\sum_{\mathbf{k}} = \int \frac{d^d k}{(2\pi)^d} = \int \nu(\epsilon) d\epsilon$

$$\Pi(0,0) = -\frac{1}{\beta L^d}\sum_{\omega_n,\mathbf{k}} \frac{1}{\omega_n^2 + (\mathbf{k}^2/2m - \mu)^2} \simeq -\frac{1}{\beta}\sum_{\omega_n}\int_{-\infty}^{\infty} d\zeta \frac{\nu(\zeta+\mu)}{\omega_n^2 + \zeta^2} \simeq -\frac{\pi\nu(\mu)}{\beta}\sum_{\omega_n}\frac{1}{|\omega_n|}$$

Introducing energy cut-off at Debye frequency $\omega_D = (2n_{\max}+1)\pi/\beta$

$$\Pi(0,0) \simeq -\nu(\mu)\sum_{n=-n_{\max}}^{n_{\max}} \frac{1}{2n+1} \simeq -2\nu(\mu)\int_0^{n_{\max}} \frac{dn}{2n+1} \simeq -\nu(\mu)\ln\left(\frac{\beta\omega_D}{\pi}\right)$$

Transition when $t/2 \equiv 1/g + \Pi(0,0) = 0$, i.e. $k_{\rm B}T < k_{\rm B}T_c = \pi\omega_D \exp\left[-\frac{1}{\nu(\mu)g}\right]$

$$\text{Near } T_c \qquad \frac{t}{2} = \frac{g}{2} - \nu(\mu)\ln\left(\frac{\beta\omega_D}{\pi}\right) - \overbrace{(g - \nu(\mu)\ln\left(\frac{\beta_c\omega_D}{\pi}\right))}^{=0}$$

$$= \nu(\mu)\ln(T/T_c) = \nu(\mu)\ln(1 + (T-T_c)/T_c) \simeq \nu(\mu)\left(\frac{T-T_c}{T_c}\right)$$

i.e. physically t is 'reduced temperature'

Lecture XXIV: †Superconductivity and Gauge Invariance

To establish origin of perfect diamagnetism and zero resistance,
one must accommodate electromagnetic field in Ginzburg-Landau Action

▷ Inclusion of electromagnetic field into BCS action: $\hat{\mathbf{p}} \to \hat{\mathbf{p}} - e\mathbf{A}$ $\qquad (c = 1)$

$$\mathcal{L}_{\rm EM} = -F_{\mu\nu}F^{\mu\nu}/4, \qquad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

Repitition of field theory in presence of vector field obtains
generalised Ginzburg-Landau theory: $\mathcal{Z} = \int D\mathbf{A} \int D[\Delta, \bar{\Delta}] e^{-S}$

$$S = \beta \int d\mathbf{r} \Big[\frac{t}{2}|\Delta|^2 + \frac{K}{2}|(\partial + i2e\mathbf{A})\Delta|^2 + u|\Delta|^4 + \overbrace{\frac{1}{2}(\partial \times \mathbf{A})^2}^{\mathcal{L}_{\rm EM}} \Big]$$

focusing only on spatial fluctuations of $\mathbf{A}$

▷ Gauge Invariance: Action invariant under local gauge transformation

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} - \partial\phi(\mathbf{r}), \qquad \Delta \mapsto \Delta' = e^{-2ie\phi(\mathbf{r})}\Delta$$

$$(\partial + i2e\mathbf{A})\Delta \mapsto (\partial + i2e(\mathbf{A} - \partial\phi))e^{-2ie\phi(\mathbf{r})}\Delta = e^{-2ie\phi(\mathbf{r})}(\partial + i2e\mathbf{A})\Delta$$

i.e. $|(\partial + i2e\mathbf{A})\Delta|^2$ (as well as $\partial \times \mathbf{A}$) invariant

▷ Anderson-Higgs mechanism:
phase of complex order parameter $\Delta = |\Delta|e^{-2ie\phi(\mathbf{r})}$ absorbed into $\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} - \partial\phi(\mathbf{r})$

$$S = \beta \int d\mathbf{r} \left[\frac{t}{2}|\Delta|^2 + \frac{K}{2}(\partial|\Delta|)^2 - \frac{m_\nu^2}{2}\mathbf{A}^2 + u|\Delta|^4 + \frac{1}{2}(\partial \times \mathbf{A})^2 \right]$$

where $m_\nu^2 = 4e^2K|\Delta|^2$

i.e. massless phase degrees of freedom $\phi(\mathbf{r})$ have disappeared!
and photon field $\mathbf{A}$ has acquired a 'mass'!

Example of a general principle:

"Below T_c, Goldstone bosons and the gauge field conspire to create massive excitations,
and the massless excitations are unobservable", cf. electroweak theory

▷ Meissner effect: minimisation of action w.r.t. $\mathbf{A}$

$$\partial \times \overbrace{(\partial \times \mathbf{A})}^{\mathbf{B}} + m_\nu^2\mathbf{A} = 0 \qquad \mapsto \qquad (\partial^2 - m_\nu^2)\mathbf{B} = 0$$

$\mathbf{B} = 0$ is the only constant uniform solution $\rightsquigarrow$ perfect diamagnetism

Free energy of superconductor first proposed on phenomenological grounds — how?
...& why is crude gradient expansion so successful?

▷ Statistical Field Theory: Ferromagnetism Revisited

Superconducting phase transition is an example of a critical phenomena

Close to the critical point, the thermodynamic properties of a system
are dictated by 'universal' characteristics

To understand why, consider simpler prototype system:
the classical Ising ferromagnet:

$$\beta H = -J \sum_{\langle ij \rangle} S_i^z S_j^z + H \sum_i S_i^z, \qquad S_i^z = \pm 1$$

Equilibrium Phase diagram?
What happens in the vicinity of critical point?

(1) First order transition — order parameter (magnetisation) changes discontinuously
correlation length remains finite

(2) Second order transition — order parameter changes continuously
correlation length diverges

...motivates consideration of "hydrodynamic" theory of classical partition function

$$\mathcal{Z} = e^{-\beta F} = \int DS(\mathbf{r})\; e^{-\beta H[S(\mathbf{r})]}$$

βH constrained (only) by symmetry (translation, rotation, etc.)

$$\beta H[S(\mathbf{r})] = \int d\mathbf{r} \left[\frac{t}{2} S^2 + \frac{K}{2} \left(\partial S\right)^2 + uS^4 + \cdots + BS \right]$$

cf. Ginzburg-Landau Theory of superconductor

Landau theory: $S(\mathbf{r}) = S$ const.

$$\frac{F(S)}{L^d} = \frac{t}{2} S^2 + uS^4$$

▷ Generally second order phase transitions divide into Universality classes
with the same characteristic critical behaviour

E.g. (1) Ising model — liquid/gas: $S \rightarrow$ density ρ, $H \rightarrow$ pressure P

E.g. (2) Superconductivity — classical XY ferromagnet

subject of statistical field theory...